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DOCTORAL THESIS

Routed quantum circuits: an extended framework for coherent control and indefinite causal order

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Author:
Augustin VANRIETVELDE

Supervisors:
Prof. Jonathan BARRETT
Prof. Giulio CHIRIBELLA
Prof. Florian MINTERT

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Declaration of Authorship

I, Augustin VANRIETVELDE, declare that this thesis titled, 'Routed quantum circuits: an extended framework for coherent control and indefinite causal order' and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while in candidature for a research degree at Imperial College London.

- Where any part of this thesis has previously been submitted for a degree or any other qualification at Imperial College London or any other institution, this has been clearly stated.

- Where I have consulted the published work of others, this is always clearly attributed.

- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.

- I have acknowledged all main sources of help.

- Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself.

Abstract

Quantum circuits form the standard framework of quantum computing, and have started playing the same role for some parts of quantum foundations. However, they cannot satisfactorily capture some possibilities offered by quantum theory, in particular coherent control and indefinite causal order. In this thesis, we therefore propose an extension to this framework, given by *routed quantum circuits*. Our extension is based on the addition of sectorial constraints, which specify the basic sectorial structure of the scenarios at hand, on top of the factorial structure described by the connectivity of circuits. This yields a consistent and scalable framework, applicable to pure and mixed quantum theory. It admits a sound and intuitive diagrammatic notation.

We show that this framework allows to properly model all forms of coherent control of the application of a channel, for instance the superposition of a quantum information carrier's trajectory, or the 'extended circuit diagrams' recently introduced for the study of causal decompositions. We demonstrate how this leads to a redefinition of the task of coherently controlling a channel, and study in detail the necessary resources for this task. We further show that the scenarios featuring indefinite causal order also fit within our framework once feedback loops are introduced. The connectivity and sectorial constraints are then sufficient to specify the core behaviour of a process, and in particular to check that it is valid, i.e. that its cycles do not lead to any logical inconsistency. We display how several standard examples of exotic processes, including ones that violate causal inequalities, are among the class of processes that can be generated in this way; we conjecture that this class in fact includes all unitarily extendible processes.

Preface

A major portion of this thesis is adapted from three publications, which were written during the course of my PhD:

1. A. Vanrietvelde, H. Kristjánsson, and J. Barrett, 'Routed quantum circuits', *Quantum* **5** (Jul, 2021) 503, `arXiv:2011.08120 [quant-ph]` [1] (Sections 2.2 and 2.3, Chapter 3, and Appendix A);

2. A. Vanrietvelde and G. Chiribella, 'Universal control of quantum processes using sector-preserving channels', *Quantum Information and Computation* **21** no 15-16 (Dec, 2021) 1320-1352, `arXiv:2106.12463 [quant-ph]` [2] (Chapter 4 and Appendix B);

3. A. Vanrietvelde, N. Ormrod, H. Kristjánsson, and J. Barrett, 'Consistent circuits for indefinite causal order', `arXiv:2206.10042 [quant-ph]` [3] (Chapter 5 and Appendix C).

In the parts mentioned, the content of these references is followed with some adaptations. The text in the remaining of this thesis is original.

I was the first author in each of these publications and contributed the majority of their key ideas. The original text of some parts was written by my co-authors, as follows:

- Hlér Kristjánsson wrote the original text that was adapted into Sections 3.2 and 5.4.2;

- Nick Ormrod wrote the original text that was adapted into Sections 5.2 and 5.4.1.

I kept these parts as they were integral to the presentation of this thesis' ideas.

Two related publications were written during the course of my PhD, which I present only briefly in this thesis:

- M. Wilson and A. Vanrietvelde, 'Composable constraints', `arXiv:2112.06818 [math.CT]` [4] (Section 6.3.1);

- N. Ormrod, A. Vanrietvelde, and J. Barrett, 'Causal structure in the presence of sectorial constraints, with application to the quantum switch', `arXiv:2204.10273 [quant-ph]` [5] (Section 6.3.2).

Finally, a presentation of my work during these three years would be incomplete without mentioning all the time I spent working on trying to prove the conjecture of causal decompositions (cf. Section 2.3). Despite its current lack of success, I do not despair that it will one day amount to something valuable.

Acknowledgements

To me, this thesis is inseparable from the wonderful time I spent in Oxford; it is indebted to all of the people who keep this city so cute and enjoyable. First among them are those who have supplied me with great food, such as Edamame, Najar's, Taylors, Ramen Kulture, Vaults & Garden, Quod, Gees, Kazbar, Arbequina, Za'atar Bake, Bannisters, Wild Honey, Missing Bean, Gail's, the East Oxford's Farmer Market, and everyone at the Covered Market and at Gloucester Green. To the Ultimate Picture Palace and its impeccable programming, I send all my gratitude for having infused life back into me during my driest moments of cerebral self-absorption.

As is the English way, there would also have been very little exchange of ideas, and very few occasions of having great fun, without the pubs; especially the Royal Oak, the King's Arms, the Turf Tavern, the Jericho Tavern, the Cape of Good Hope, the Half Moon, and – I shamefully admit – the Old Black Horse.

I was lucky enough to live in a fine house with awesome people. Nicole, Liam, Daniel and Nicolas were always there to talk for hours about our academic and personal lives, to cheer me up when I was grumpy, to watch a good movie, to endure my jokes about John Skinner, and to have great meals and nights out. It was a wonderful feeling knowing every day that I would come back in the evening to a lively and caring home. I will miss you guys!

Paying for the rent in this house and the beers in these pubs was the Engineering and Physical Sciences Research Council (EPSRC), through its funding of the "Controlled Quantum Dynamics Centre for Doctoral Training" (CQD CDT). Surely behind these acronyms there are invisible actual people, who do the dirty job of getting us the money. I thank them dearly for making all of this possible.

At an intermediate level, this thesis was also made possible by the involvement of people at Imperial, especially Ben and Myungshik, to secure the existence of the CQD CDT. I thank them for that, as well as Miranda, for her swiftness and competence in all administrative tasks – something that I fear I will rarely encounter again. I am also indebted to my cohort in the CDT for having made our year of Masters nice and enjoyable. Special thanks go to Hadrien, as well as Esther and Timmy, for their support and great conversations during this first year and beyond.

A person I never met or even talked to, but whose involvement has significantly improved my life as well as that of countless other people, is Alexandra Elbakyan. I thank her for her courage in standing up to monopolisation and parasitism, and I wish her luck for the future of her fight.

After eighteen months of covid, it is hard to overstate how important it has been both for my scientific ideas and for my mental wellbeing to be able to attend conferences and exchange ideas with incredibly gifted and imaginative people. My deepest gratitude goes in particular to the organisers of the Sejny 2021 conference, which has been a life-changing event. I also thank the organisers of the wonderful conferences in Hong Kong, Paris, London, Oxford, Lesbos and Zurich, as well

To my father.

For what use will it be on the Day of Judgment, when all human achievements are weighed, to offer up three articles on formic acid, or even thirty? On the other hand, what do we know of the Day of Judgment if we do not even know what may have become of formic acid by then?

Robert Musil, *The Man without qualities*.

A life of route.

Black M.

Chapter 1

Introduction

When, at the turn of the nineties, a few pioneers set out to chart the unexplored territory of quantum computing, their enterprise did not start with the discovery of the specific quantum algorithms that would draw significant attention to the field. First, they had to define what quantum algorithms even *were*, to delineate the class they formed, the world in which they lived. This is what led Deutsch, in a 1989 paper, – three years before discovering the first quantum speedup with Jozsa –, to propose the language of *quantum circuits* [6].

The remarkable ensuing fortune of quantum circuits – and of their subsequent refinements and reformulations [7–11] – has much to do with their success in providing a *framework*. As such, they define a common language within research: they formally designate what is and is not a legitimate object of study, and offer tools to compare these objects in an unambiguous and quantitative way [10]. They also come with convenient structural properties that allow one to handle these objects in an intuitive way, and in particular with the help of graphical reasoning [11].

As an evident generalisation of the logical circuits of classical computing, with which computer scientists were familiar already, quantum circuits naturally came to shape the whole field of quantum computing. But their influence did not stop there. It gradually appeared that in his definition, Deutsch had done little more than stripping quantum theory of its 'physical' part – if by 'physical' we mean specific discussions of atoms, electrons, spins, momenta, and the rest – and exposing its bare informational bones for everyone to see. This conceptual asceticism was especially attractive to the practitioners of quantum foundations. With time, quantum circuits quietly bounced back into physics. They started their life as an informational coarse-graining, a property to be derived from a fundamental physical model; to some, they have now become the fundamental model itself, the central skeleton whose fleshing-out into a fully formed physical situation – involving electrons, atoms and the rest – appears more and more insignificant.[1]

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[1]Of this fascinating transformation, which is only at its infancy and still confined to a subfield of physics, much more could be said, which we unfortunately do not have the time to expand on here. Let us simply note that this is just the compositional (or, to put it more boldly, the spatiotemporal) facet of a wider shift: the ongoing Copernican revolution generated by the re-examination of quantum theory in the light of informational notions. It is also worth mentioning that the 'quantum circuits' shift in perspective is inseparable from the adoption – be it at a conscious or unconscious level – of the point of view of *process theories* (cf. Section 2.1.1).

As with many conceptual schemes, however, the success of quantum circuits carried the seeds of their eventual ailments. There were two main ones. First, the mental shift we reported, through which more and more physical situations came to be regarded as quantum circuits, led to a disturbing realisation. This took the form of a no-go theorem, stating the impossibility for any quantum circuit to implement the coherently controlled version of an unknown unitary evolution [12, 13]. What made the situation awkward is that physical architectures *had* already been built that achieved just this; all one had to do was to use superpositions of trajectories [14]. The fault, it seemed, was with the quantum circuits framework within which these no-go theorems were stated, and its incapacity to properly model this standard quantum situation [13].

The second issue emerged as a result of a systematic effort to mathematically characterise the action of quantum circuits [10, 15]. It was then realised that one of the mathematical assumptions in this characterisation – related to the acyclicity of the evolutions' ordering – could be dropped, leading to intriguing possibilities, that have been characterised as featuring 'indefinite causal order' [16–18]. At least some of these seem to be realisable experimentally, and indeed the simplest is claimed to have been realised [19–24], although this has spurred much debate. From a practical point of view, their use could unlock advantages over standard quantum architectures, in many tasks [25–41]. By definition, these exotic scenarios cannot be framed as quantum circuits.

Both of these situations have led to the existence of 'out-of-framework scenarios'.[2] This is a precarious state of affairs, bound to spark – and which indeed has sparked already [22, 34, 42–49] – strenuous controversies over the legality of the scenarios themselves, the applicability of any given investigation of their properties, or the commensurability of these properties. In contrast with intra-framework discussions, these out-of-framework controversies cannot rely on a generally accepted notion of what the 'correct' analysis is; participants have to fall back on contextual arguments whose conceptual premises might not be shared in the community. These questions cannot be conclusively settled until the scenarios are integrated into a new framework; until then, we will be battling with the fog.

Can we, then, design a general, pliable, and trustworthy informational framework in which these stray scenarios can be accurately described? To this question, this thesis answers in the affirmative.

One thing might lead to confusion about what we achieve: there are different, interdependent manners in which one could claim to have provided a framework here. A particularly critical and much acknowledged one is to provide a clear conceptual

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[2]To be precise, architectures with indefinite causal order do fit within the framework of superchannels (or equivalently, of process matrices), obtained by the assumption-dropping we just described. But this is an extremely opaque and unwieldy framework, that ought to be refined into a more descriptive one. Note also that coherent control scenarios can be shoehorned into the framework of quantum circuits, but at the cost of considerable distortion. We expand on all of this in great detail in Chapter 2.

link between the *informational* and the *physical* descriptions; or in other words, to unambiguously specify which physical situations constitute legal implementations of a given theoretical process. (In our opinion, this demanding objective has not been fully met even in the case of standard quantum circuits.) Important work in this direction has been produced already [50–54]. We want to stress that this kind of an 'informational-to-physical' framework is *not* what we are considering here.

Indeed, our framework remains fully at the informational level: it models processes in the abstract, describing operations and systems that do not carry a specific physical interpretation, for examples in terms of spacetime locations. (This will not forbid us from mentioning specific physical interpretations as illustrations, in order to build up intuition.) Perhaps surprisingly, even this more modest task turns out to be somewhat non-trivial. In our view, carrying it out is a prerequisite to any successful clarification of the 'informational-to-physical' question.

How, then, should we extend the framework of quantum circuits? Our solution takes inspiration from the insights and techniques of two recent works, stemming from two seemingly independent lines of research. The first one [55] informally introduced 'extended quantum circuits' in order to spell out a tentative equivalence between the causal and compositional structures of unitary transformations. The second [56] put forward a new description of the previously mentioned 'superposition of trajectories' scenario, in order to propose a well-defined analysis of its communicational properties. Remarkably, both works achieve their goals by leveraging on the same fundamental structure of quantum theory, which lies at the foundation of our model.

To describe this structure, it is profitable to contrast it with a familiar one. In quantum theory, *factorial* structure, mathematically described by a tensor product structure, is the counterpart to our intuitive notion of 'splitting into parts'. These parts correspond to *factors* of the global system. By construction, quantum circuits are particularly well-adapted to the description and manipulation of factorial structure: it appears directly in their defining axioms, and is conveniently represented by parallel composition. Accordingly, its handling has become intuitive and natural to most practitioners.

Another important structure, however, is given much less visibility: *sectorial* structure, the quantum counterpart to our intuitive notion of 'splitting into alternatives', mathematically described by a direct sum structure. These alternatives then correspond to *sectors* (i.e. orthogonal subspaces) of the global system.[3] In sharp contrast to factorial structure, sectorial structure is pretty much invisible in quantum

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[3]'Alternative' here is of course to be understood in a quantum way, allowing for superpositions; the same could be said about the above 'parts', which allow for entanglement. We do not want to imply that sectors/factors match our classical notion of alternatives/parts; we simply note that they are their quantum analogues at a conceptual level.

circuits. Consequently, it is often difficult to reason intuitively about it.[4]

Fundamentally, what Refs. [55] and [56] do can be summed up in simple terms: they spell out the existence of some crucial sectorial structure in the specific scenarios they are dealing with. The manner in which they do so can be conceptualised as the introduction of *sectorial constraints*: constraints on dynamical evolutions, encoding the fact that these evolutions do not connect some sectors of their input and output spaces. Introducing sectorial constraints is essentially a way of rendering the sectorial structure that had been neglected in standard circuits. Conversely, the failure of the latter to encompass the stray scenarios can be regarded as a consequence of this neglect.[5]

And indeed, this thesis shows that the incorporation of sectorial constraints is the only required ingredient to build an extended framework that properly includes most of our stray scenarios: all of the ones stemming from coherent control, and a significant chunk (which we conjecture to be the unitarily extendible subset [59]) of the ones featuring indefinite causal order. (This includes some that violate causal inequalities, essentially meaning that they are exotic in a strong way.) In particular, our elementary addition brings together these two types of deviations within a unified framework. Because we formally encode sectorial constraints using objects called *routes*, the resulting framework is called *routed quantum circuits*. Routed quantum circuits are scalable, pliable, and intuitive, as any framework ought to be; furthermore, they give rise to an intuitive diagrammatic depiction in terms of decorated circuits.

Routed quantum circuits are the relevant informational framework in which the full scope of scenarios allowed by quantum control and indefinite causal order can be described, with the exception of some highly exotic processes for which even a tentative physical implementation has never been put forward. We expect that their use will provide the common ground on which discussions of these scenarios and their properties can be solidly and safely set. We hope the informational framework they constitute can be fruitfully joined with the current attempts at the design of 'informational-to-physical' frameworks, by clarifying their starting point.

Because they allow us to contemplate the full width of possibilities offered by quantum theory, routed quantum circuits could also facilitate the design of new ones, or trigger the 'rediscovery' of existing ones which, much like the superposition of trajectories, had been overlooked or put aside because they could not be framed within the standard framework. In our view, the most appealing prospect would be for them to play a part in the slow movement that has been quietly driving our field from beneath the surface: the rejuvenation of our fundamental physical concepts in the light of an informational perspective.

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[4]In our own experience, we have often been surprised with the amount of confusion – especially confusion with the factorial structure – that the examination of sectorial structure initially elicits in many people, starting with ourselves.

[5]On the subject of sectorial structure, we have to pay tribute to the prescient work of Johan Åberg back in 2004 [57, 58], which was completely ignored by his contemporaries.

Outline

We start by discussing in detail the motivation for the introduction of our extended framework (Chapter 2). This amounts to a presentation of the deficiencies of the framework of quantum circuits. After presenting the latter in a way that puts emphasis on its compositional structure (Section 2.1), we study three subjects for which it proves ill-suited: superpositions of trajectories (Section 2.2), causal decompositions (Section 2.3), and indefinite causal order (Section 2.4). We also use this opportunity to introduce the crucial ideas that will be leveraged in our construction, especially in Sections 2.2 and 2.3.

We then present routed quantum circuits, first restricting ourselves to scenarios that do not feature indefinite causal order (Chapter 3). We present the framework for pure quantum theory (Section 3.1) and discuss its diagrammatic representation (Section 3.2), before extending it to noisy quantum theory (Section 3.3). We finally show how the 'extended quantum circuits' of Ref. [55] form a sub-framework, called *index-matching quantum circuits*, that enjoys a particularly handy diagrammatic representation (Section 3.4).

In Chapter 4, as an interlude, we entertain the reader with an application of our framework. Specifically, we show how its conceptual and formal ideas yield a clarification of the long-standing misapprehension of the problem of coherent control. After a presentation of the relevance of this computational problem and the current state of the literature (Section 4.1), we discuss the general form of coherently controlled channels (Section 4.2) and the nature of the resource with which they can be implemented (Section 4.3). We then display the universal computational architecture that turns this resource into a corresponding controlled channel (Section 4.4), and extend our discussion to the coherent control between multiple channels (Section 4.5). Finally, we show how the architectures realising these tasks can be understood formally as *supermaps on routed channels*, or routed superchannels (Section 4.6).

Turning to the case of indefinite causal order, we show how routed quantum circuits with feedback loops can be used to capture it as well (Chapter 5). After a discussion of the specific challenges and goalposts on that matter (Section 5.1), we first introduce our framework with a pedagogical presentation of how it applies to the quantum switch (Section 5.2), before presenting it in formal detail (Section 5.3). We show how this framework allows to reconstruct several standard examples of exotic processes (Section 5.4) and end with a discussion of these results (Section 5.5).

We conclude our thesis in Chapter 6, by providing a short summary (Section 6.1), discussing the limitations of the framework as it is currently defined (Section 6.2), briefly reviewing related work we have carried out on this subject (Section 6.3), and mentioning some possible avenues for future research (Section 6.4).

As for the Appendices, we strongly advise the reader valuing their mental sanity not to venture into them.

Chapter 2

Background and motivation

> *With use, ideas take on unwarranted* value. *A value in itself impedes the circulation of values. It is a factor of inertia for the mind. (. . .) An irreverent epistemologist said, some twenty years ago, that great men are useful to science in the first half of their lives and harmful in the second.*
>
> Gaston Bachelard, *The Formation of the Scientific Mind*.

In our introduction, we made some serious allegations against quantum circuits, claiming that they had proved unable to satisfactorily model some of the possibilities offered by quantum theory. In this chapter, we will back this point in detail.

We will start (Section 2.1) by spelling out a formalisation of quantum circuits as a theory. We will then describe the subject and results of three areas of research in quantum theory (Sections 2.2, 2.3 and 2.4) and discuss the sense in which they lead us beyond this paradigm.

2.1   The standard: quantum theory as a circuit theory

In this section, we review the standard framework of quantum theory. By 'standard framework', we essentially mean the framework of quantum circuits, in which operations are causally ordered, and in which no sectorial constraints or correlations are present. The aim of this presentation is to provide a backdrop against which to contrast the non-standard scenarios that we will then display.

In broad terms, what characterises these non-standard scenarios is their unusual compositional features. To get a sharp contrast, it would thus be fitting for us to start with a presentation of the standard framework that stresses its compositional structure. A natural way to do this is to use the language of *process theories*. For this purpose, we will largely follow the presentation of the standard reference [11].[1] As a proper introduction would be way too long, we will skip a lot of details and focus on the main intuition.

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[1] In general, we warmly recommend this reference to anyone with interest in the subject.

2.1.1   The basics of process theories

Before we look at quantum theory in particular, let us lay down the basics. A process theory is a theory of processes and of how they compose. The central notion is that of a process (also called a *map* or a *morphism*), by which we mean, something with an input and an output. For instance, one could have a process $f : A \to B$ (i.e. with input A and output B). This has a natural diagrammatic representation as a box with an input wire A and an output wire B,

$$\begin{array}{c} \vert B \\ \boxed{f} \\ \vert A \end{array} . \tag{2.1}$$

To give our example of a process, we also had to refer to instances of the other critical notion of process theories: the things A and B between which f maps. Depending on the context, these are called *system-types* or *objects*; alternatively, the unfamiliar reader can broadly think of them as corresponding to the usual notion of a space (e.g. a set, a vector space, a manifold, etc.). Objects and maps are the two pillars of process theories.

In a process theory, one can compose maps in sequence, as long as their types match. For example, if we have $f : A \to B$ and $g : B \to C$, then from them we can form a map $g \circ f : A \to C$. Diagrammatically, this has a natural representation in which we plug one box into the other:

$$\begin{array}{c} \vert C \\ \boxed{g} \\ \vert B \\ \boxed{f} \\ \vert A \end{array} . \tag{2.2}$$

In a process theory, the composition $\circ$ is associative and admits unit elements, given by identities: on each object A, there exists a map $\mathrm{id}_A : A \to A$ satisfying $g \circ \mathrm{id} = g$ and $\mathrm{id} \circ f = f$ for any map. In diagrams, identities are represented by pieces of wires, matching the intuition that they don't do anything. With these features, our process theory corresponds to the technical notion of a *category*.

The next step is to make way for a notion of parallel composition, capturing the intuition of 'doing things in parallel'. This parallel composition $\otimes$[2] acts both on objects, forming $A \otimes B$ from A and B, and on processes, forming $g \otimes f : A \otimes C \to B \otimes D$ from $f : A \to B$ and $g : C \to D$. This has a natural diagrammatic representation in which the processes are put next to each other,

---

[2]Note that, even though we use the symbol $\otimes$, at this point this parallel composition is just an abstract notion, and doesn't have to be a tensor product.

$$
\begin{array}{cc}
\!\!\!\!\mid B & \mid D \\
\boxed{f} & \boxed{g} \\
\mid A & \mid C
\end{array}
\qquad\qquad . \tag{2.3}
$$

To ensure that our parallel composition is reasonably well-behaved, we ask for $\otimes$ to be associative, to distribute over the sequential composition, and to have a unit element – i.e., there exists a 'unit object' I such that $A \otimes I = I \otimes A = A$, and $f \otimes \mathrm{id}_I = f$.[3] One can think of I as a trivial space corresponding to a trivial system (typically, $\mathbb{C}$ in the theory of complex linear maps); diagrammatically, it can be represented as a blank space, as putting a blank space next to a diagram doesn't change anything.

Finally, one asks for the existence of swaps allowing one to change the order of objects (e.g. $\mathrm{SWAP}_{A,B} : A \otimes B \to B \otimes A$), together with a few other natural conditions ensuring that the previous notions play together in the expected way. This yields what we will call a *circuit theory*.[4] As the name indicates, the main point of circuit theories is that they are subject to the following theorem. What we mean by a circuit here is a causally ordered wiring of processes, without feedback loops,[5] that can be built recursively by using sequential and parallel composition of the processes.

Theorem 2.1.1. *[11, 60] Circuit theories admit a sound and complete representation in terms of circuit diagrams.*

Soundness in Theorem 2.1.1 means the following. We take two circuit diagrams whose wires are objects of the theory and whose boxes are morphisms; if these are equal as diagrams (i.e. if one can be obtained by simply deforming the other), then the processes they represent are provably equal [11]. Essentially, this should be understood as ensuring that circuit diagrams can be used without second thoughts when dealing with a circuit theory: all the natural intuitions that these diagrams lead to are warranted by the theory's compositional structure.

Completeness means, on top of this, that the language of diagram deformation allows one to infer *all* of the equalities that could be proved using the axioms of circuit theories. In other words, circuit diagrams represent precisely the structure of circuit theories: there is nothing we miss of that structure by using them.

To give some intuition, a typical example of a process theory that will be relevant to us is that of finite-dimensional complex linear maps. In this theory, objects are Hilbert spaces, maps are linear maps between them, parallel composition is the

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[3]In all rigour (and this will also apply later in this section), the equal signs in these equations should rather be written as isomorphisms, e.g. $I \otimes A \cong A$. Dealing with these isomorphisms would require going to a level of technicality that would blur the main conceptual points, without much purpose in the context of the applied picture we care about in this thesis. We will therefore overlook this and apply the slogan: 'mathematicians did it so we wouldn't have to'.

[4]In technical terms, this is a symmetric monoidal category.

[5]Ironically, this is in fact in total contradiction with the everyday notion of a circuit, which commonly refers to closed loops, as indicated by the etymological connection to 'circle'. For this reason, circuits are sometimes called *networks* instead; this is for example the terminology of Deutsch's seminal paper on quantum computation [6].

tensor product, and the unit object is the trivial Hilbert space $\mathbb{C}$. In the same way that Monsieur Jourdain has been speaking prose all his life without knowing it, anyone using linear maps is inadvertently doing heavy category theory.

An important point to understand is how states (and effects) are recovered. Indeed, one might worry that in a process theory one has defined maps without ever talking about the things that these maps transform. The remarkable feature is that states do, in fact, exist in circuit theories: they are simply special cases of processes. Specifically, a state on an object A is just a map $\psi : I \to A$, where I is the unit object that we already encountered. Diagrammatically, because I is just a blank space, one gets the intuitive picture of a map without any input, usually depicted as a triangle:

$$
\begin{array}{c} | A \\ \triangledown_\psi \end{array} \quad := \quad \begin{array}{c} | A \\ \boxed{\psi} \\ \vdots\, I \end{array} \; . \tag{2.4}
$$

To give some intuition, one can think of the fact that a state in the theory of complex linear maps, generally defined as an element of a Hilbert space $\mathcal{H}$, can equivalently be seen as a map $\mathbb{C} \to \mathcal{H}$. In that sense, the framework of process theories turns on its head the standard conceptual view on maps, in which static 'things' (such as elements of a set) are presented as conceptually prior, and maps are seen as a derived concept from them, as 'what takes a thing and produces another thing'; here, on the contrary, maps are conceived in the abstract, and 'things' – i.e. states – are derived as specific instances of maps.

Symmetrically, one can define effects on an object A as the maps $A \to I$ (the intuitive example is that of a bra in the theory of complex linear maps), depicted diagrammatically as upside-down states. Finally, the maps $I \to I$ are called *scalars* (in the theory of complex linear maps, these will be the complex numbers), usually depicted as boxes with no incoming or outgoing wires. To give an intuition of why this makes sense, one can think of the diagram

$$
\begin{array}{c} \triangle_\phi \\ | \\ A \\ | \\ \triangledown_\psi \end{array} \tag{2.5}
$$

as a scalar itself, as the whole diagram has no inputs or outputs: in the theory of complex linear maps, this will precisely be the complex number $\langle \varphi | \psi \rangle$.

One might wonder whether it is possible to go further and allow feedback loops as well. To get this, we need to ask our circuit theory to features, for each object A, a dual object A^*, a specific state on $A \otimes A^*$ called the *cup*, and a specific effect on $A^* \otimes A$ called the *cap*, diagrammatically depicted as bendings of a wire,

$$\bigcup \quad := \quad \bigtriangledown_{\cup} \quad , \tag{2.6a}$$

$$\bigcap \quad := \quad \bigtriangleup^{\cap} \quad , \tag{2.6b}$$

and satisfying the so-called *yanking equations*,

$$\tag{2.7a}$$

$$\tag{2.7b}$$

$$\tag{2.7c}$$

together with a few other natural conditions that ensure that they play well with the rest of the theory's structure. To give intuition, in the theory of finite-dimensional complex linear maps, cups and caps correspond to the Bell state's (unnormalised) ket and bra, respectively. In a statement analogous to Theorem 2.1.1, theories featuring such structure (corresponding in technical terms to compact closed monoidal categories) admit a sound representation in terms of *string diagrams*, i.e. 'circuit diagrams with feedback loops' [11]. This should once again be understood as ensuring that one can then reliably use such diagrams and the intuition they contain.[6]

2.1.2 The case of quantum theory

When studying quantum information, one is led to use four related process theories: that of complex linear maps, that of the isometric maps among them (i.e. 'pure quantum theory'), that of completely positive complex linear maps, and that of the trace-preserving maps among them (i.e. 'mixed quantum theory'). We will discuss

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[6]In fact, in order to make sense of feedback loops that only link outputs to inputs, one only requires a weaker notion, that of a traced monoidal category.

their respective features in the light of the previous considerations. For simplicity, we will entirely restrict ourselves to the case of finite dimension.

In each of these theories, objects A correspond to (finite-dimensional) Hilbert spaces $\mathcal{H}_A$. In complex linear maps, the processes $A \to B$ are the linear maps $f : \mathcal{H}_A \to \mathcal{H}_B$. In pure quantum theory, they are the linear maps $U : \mathcal{H}_A \to \mathcal{H}_B$ satisfying $U^\dagger \circ U = \mathrm{id}_A$. In completely positive linear maps, they are the completely positive linear maps $\mathcal{E} : \mathrm{Lin}\,[\mathcal{H}_A] \to \mathrm{Lin}\,[\mathcal{H}_B]$. Finally, in mixed quantum theory, they are the completely positive linear maps $\mathcal{C} : \mathrm{Lin}\,[\mathcal{H}_A] \to \mathrm{Lin}\,[\mathcal{H}_B]$ satisfying $\forall \rho \in \mathrm{Lin}\,[\mathcal{H}_A]\,, \mathrm{Tr}\,[\mathcal{C}(\rho)] = \mathrm{Tr}\,[\rho]$.

Note that complex linear maps embed into completely positive maps, through the mapping of $f : \mathcal{H}_A \to \mathcal{H}_B$ to $\hat{f} : \mathrm{Lin}\,[\mathcal{H}_A] \to \mathrm{Lin}\,[\mathcal{H}_B]$ acting as $\hat{f}(\cdot) = f \circ \cdot \circ f^\dagger$. The same mapping embeds pure quantum theory into mixed quantum theory. In that sense, one can see the former as a sub-theory of the latter.

Each of these four theories forms a circuit theory, with the parallel composition given in each case by the tensor product [11]. This warrants the use of circuits in (pure or mixed) quantum theory, as Theorem 2.1.1 ensures that these are sound; in other words, it is always possible to perform any quantum operations in a causally ordered way.

What about feedback loops? A first thing to note is that these do make sense in linear maps and in completely positive maps. Indeed, in each of these theories, the (unnormalised) Bell state yields a cup and a cap with the required properties. Note that in completely positive maps, compact closure (i.e. the existence of cups and caps) is widely known as the *Choi-Jamiołkowski isomorphism* [61, 62]. Indeed, one of the ways to see compact closure is that it yields a *process-state duality*: processes $A \to B$ are in one-to-one correspondence with states on $A^* \otimes B$, via

$$
\begin{array}{c}
\begin{array}{|c|} \hline B \\ \hline f \\ \hline A \end{array}
\end{array}
\quad \simeq \quad
\begin{array}{c}
A^* \quad \begin{array}{|c|} \hline f \\ \hline \end{array} B \\
 A
\end{array}
\quad .
\tag{2.8}
$$

The Choi-Jamiołkowski isomorphism is the application of that duality to completely positive maps, which find themselves in a one-to-one correspondence with states (i.e. positive maps) on the tensor product of their output space with the dual of their input space.

These feedback loops, however, do not fit into either pure or mixed quantum theory. This is because 1) the cup is not normalised, and 2) more importantly, the cap is not a valid deterministic quantum process, even up to renormalisation – in fact, there are no valid effects in pure quantum theory except for scalars, while in the mixed theory the only allowed effect is the discarding effect. It is thus in general not possible to make sense of string diagrams in either pure or mixed quantum theory.[7]

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[7]Except of course if one allows probabilistic implementations; but the meaning would then be starkly different.

This concludes our (very introductory) overview of quantum theory's compositional structure, when formalised using quantum circuits. In the rest of this Chapter, we will consider scenarios whose proper formalisation, as we shall argue, requires to go beyond this standard structure. Two aspects will in particular be challenged: the fact that parallel composition should always correspond to a tensor product, and the fact that only a non-cyclic ordering of operations should be allowed.

2.2 Superpositions of trajectories

Our first case of study is the 'superposition of trajectories' scenario. We will present it and argue that under certain natural requirements, this scenario cannot be properly formalised within the standard picture, specifically because the tensor product is not the relevant parallel composition. This will also allow us to introduce the concepts of sectorial constraints and sectorial correlations, which will be central to this thesis.

2.2.1 The scenario

The study of communication in a superposition of trajectories was recently proposed as a framework that extends standard quantum Shannon theory [49, 56]. In this framework, not only is the information carried by a message that is allowed to be in a quantum state, but also the trajectory of the quantum information carrier is allowed to be in a coherent superposition of different transmission lines. The goal of Refs. [47, 56] was to study the communication advantages that using such scenarios can lead to. In a similar spirit, several recent works have investigated the use in quantum computation of controlling unknown 'black box' quantum operations, where a quantum control system determines if one unknown operation is used, or another, or both in a superposition [12–14, 63–66]. What matters to us here are the challenges that these works raise in terms of mathematical formalisation. To introduce them, we will focus on a paradigmatic example of communication in a superposition of trajectories, the 'one message in two trajectories' scenario [47, 56], focusing specifically on the perspective of Ref. [56].

Even though we will focus on this specific example in order to present sharp arguments about a well-defined situation, the following analysis applies to a wide range of quantum-optical or interferometric setups to show that, in general, they cannot be faithfully described by standard quantum circuits. Indeed, the features of this example are ubiquitous in quantum optics, in which sending a photon in a superposition of trajectories, and applying operations that do not modify the number of photons (such as waveplates) are standard protocols. This point has, in particular, been encountered in different guises in the literature discussing the possibility of coherently controlling unknown unitaries [13, 14, 63, 64] or quantum channels [47, 56–58, 65–68]: no-go theorems forbid such coherent control in standard quantum circuits, yet it is achievable in simple quantum optical implementations. This

is because these quantum optical implementations of coherent control of quantum channels cannot be correctly described by standard quantum circuits.[8]

(The specific problem of coherently controlling an unknown unitary, and more generally an unknown channel, will be discussed later in this thesis, in Chapter 4. Indeed, our analysis of it will build on the formalisation of the superposition of trajectories introduced in Chapter 3, confirming that the two problems are deeply interlinked.)

Going back to our main example, let us describe it in informational terms. There is a sender S and a receiver R, and there are two different communication lines from S to R. These communication lines, A and B, can be thought of as being under the control of two agents, Alice and Bob. The sender wants to transmit a qudit message[9] M, and there is an additional control qubit C, whose value coherently determines whether the message goes through Alice's or Bob's communication lines. The agent that does not get the message is instead handed a 'vacuum state', orthogonal to the possible states of the message.[10] The agents' operations cannot affect whether there is a message in their communication lines – i.e. they can only map a message state into a message state, and the vacuum state into itself. Afterwards, the two communication lines are merged back, yielding again a message and a control qubit for the receiver to analyse.

A mathematical description of this scenario is the following. The communication lines are represented as quantum channels (i.e. CPTP maps) $\mathcal{A}$ and $\mathcal{B}$, acting on $\mathrm{Lin}(\mathcal{H}_A)$ and $\mathrm{Lin}(\mathcal{H}_B)$, where $\mathcal{H}_A$ and $\mathcal{H}_B$ are Hilbert spaces of dimension $d+1$. Moreover, each of these Hilbert spaces is partitioned into two orthogonal subspaces (also called sectors): a one-dimensional subspace corresponding to the vacuum state (the vacuum sector), and a d-dimensional subspace corresponding to the possible states of the message (the message sector). This partitioning (or sectorisation) is written as

$$\mathcal{H}_A = \mathcal{H}_A^0 \oplus \mathcal{H}_A^1 \,, \tag{2.9a}$$

$$\mathcal{H}_B = \mathcal{H}_B^0 \oplus \mathcal{H}_B^1 \,. \tag{2.9b}$$

---

[8]On this point, see in particular the discussions in Refs. [13] and [63]. Ref. [13] concludes that 'the language of quantum circuits should be extended in order to capture all information processing possibilities allowed by quantum physics': we see this as an apt forecast of the work undertaken in the present thesis, which precisely describes such an extension. Ref. [63] argues that implementations of coherent control can be represented using standard quantum circuits, but that 'the correct circuit representation of a schematic may not resemble it visually'; in terms of our requirements for 'adequate representations', this entails that this representation in standard quantum circuits will be inadequate. This is because it does not neatly distinguish the subsystem on which the operation to be controlled is acting, as we discuss below.

[9]This message is also sometimes called a particle. However, we do not want to commit to any physical interpretation: to us, the message is a purely informational concept and could be physically instantiated by any type of a localised degree of freedom.

[10]Here as well, we want to stress that to us, the 'vacuum' is a purely informational concept, that should not be confused with the physical vacuum of e.g. Fock spaces or quantum field theory, even though the two notions will coincide in most implementations. 'Vacuum' here simply means 'absence of the message'; the role of embodying this absence could be played by many physical states, as long as they are orthogonal to the possible states of the message.

$\mathcal{A}$ and $\mathcal{B}$ are constrained to map the vacuum sector to itself, and the message sector to itself. This is called the *no-leakage condition* in Ref. [56]; in this thesis we will pin down such constraints under the name of *sectorial constraints*, i.e. constraints on which input sector may be mapped to which output sector. Finally, initialisation of the trajectories' superposition is described by a unitary channel $\mathcal{U}$ from $\mathrm{Lin}(\mathcal{H}_M \otimes \mathcal{H}_C)$ to $\mathrm{Lin}(\widetilde{\mathcal{H}}_{AB})$, where

$$\widetilde{\mathcal{H}}_{AB} := \mathcal{H}_A^1 \otimes \mathcal{H}_B^0 \ \oplus \ \mathcal{H}_A^0 \otimes \mathcal{H}_B^1 \tag{2.10}$$

is the 'message' subspace of $\mathcal{H}_A \otimes \mathcal{H}_B$, that excludes $\mathcal{H}_A^0 \otimes \mathcal{H}_B^0$ ('no one receives a message') and $\mathcal{H}_A^1 \otimes \mathcal{H}_B^1$ ('both receive a message').

The peculiar way in which $\widetilde{\mathcal{H}}_{AB}$ is built out of specific combinations of $\mathcal{H}_A$'s and $\mathcal{H}_B$'s sectors in (2.10) is an instance of a feature that will prove important to us. We will call this feature *sectorial correlations*, i.e. correlations between which sector is populated in A and which is populated in B.

The termination of the superposition is given by $\mathcal{U}^\dagger$ (depending on the specification of the scenario, it could also be given by any other unitary channel from $\mathrm{Lin}(\widetilde{\mathcal{H}}_{AB})$ to $\mathrm{Lin}(\mathcal{H}_M \otimes \mathcal{H}_C)$). Note that this scenario is consistent because of the crucial requirement that the vacuum and message sectors are preserved by $\mathcal{A}$ and $\mathcal{B}$, as otherwise $\mathcal{A} \otimes \mathcal{B}$ wouldn't map $\mathrm{Lin}(\widetilde{\mathcal{H}}_{AB})$ to itself.

We now show the kind of description of this scenario that standard quantum circuits yield. Given that Alice and Bob's channels are applied in parallel and in different regions of spacetime, a natural diagrammatic representation of this scenario should have the following form (here, $\mathcal{E}$ stands for 'encoding' and $\mathcal{D}$ for 'decoding'):

$$\tag{2.11}$$

In a quantum circuit, the boxes here correspond to CPTP maps, and the wires correspond to spaces of linear operations on Hilbert spaces. The conjunction of wires A and B corresponds to the space $\mathrm{Lin}(\mathcal{H}_A \otimes \mathcal{H}_B)$. We see that this description as a standard quantum circuit depicts neither sectorial correlations (here, the fact that B gets the vacuum state if A gets the message, and reciprocally) nor sectorial constraints (here, the fact that $\mathcal{A}$ and $\mathcal{B}$ have to preserve the existence or not of a message).

2.2.2 Why are standard circuits inadequate?

We now argue that this standard description is inadequate and should be refined. As this point is central to motivate the introduction of our extension to quantum

circuits in Chapter 3, we will justify it in detail, spelling out precisely the notion of adequacy that leads us to this conclusion, as well as the rationale for upholding this notion of adequacy.

Oversized Hilbert spaces

A good way to start is with some straightforward comments on the fact that (2.11) does not include key elements of the scenario, and in particular sectorial correlations. For example, $\mathcal{E}$ is a map to $\mathrm{Lin}(\mathcal{H}_A \otimes \mathcal{H}_B)$, and not to its subspace $\mathrm{Lin}(\widetilde{\mathcal{H}}_{AB})$, even though the latter is the sector that will always be used in this scenario, no matter Alice and Bob's choices of operations. In general, one is forced to manipulate Hilbert spaces that are 'too big' in comparison with the Hilbert spaces in actual use. Such a looseness implies, for example, that $\mathcal{D}$ cannot be taken to be equal to $\mathcal{U}^\dagger$, as the latter has input space $\mathrm{Lin}(\widetilde{\mathcal{H}}_{AB})$ and is therefore not trace-preserving if extended to $\mathrm{Lin}(\mathcal{H}_A \otimes \mathcal{H}_B)$. To make $\mathcal{D}$ trace-preserving, one will have to incorporate to it, on top of $\mathcal{U}^\dagger$, elements that specify how it acts on the other sectors of $\mathrm{Lin}(\mathcal{H}_A \otimes \mathcal{H}_B)$, even though this is irrelevant information as far as the scenario is concerned.

That (2.11) does not explicitly include sectorial constraints either – i.e. the requirement that the agents cannot alter the fact of whether or not there is a message in their communication line – is in fact related to its omission of sectorial correlations. Indeed, as we noted, the inclusion of the constraints is crucial to ensure the persistence of the correlations: it is because of the sectorial constraints that we know that $\mathcal{A} \otimes \mathcal{B}$ maps $\mathrm{Lin}(\widetilde{\mathcal{H}}_{AB})$ to itself, and not to elsewhere in the 'big' space $\mathrm{Lin}(\mathcal{H}_A \otimes \mathcal{H}_B)$.

So, roughly speaking, what characterises the standard description (2.11) is that it features oversized Hilbert spaces. That this, at least for certain purposes, makes it inadequate, is what we will now demonstrate.

Invariants and variables

The point of our formalisation is to be able to track how the input system (i.e. the message and the control qubit taken together) evolves along the protocol. In particular, in the middle of the protocol, this system has transformed into the (isomorphic) system of 'a message in the possession of Alice and Bob'. Yet this is not what (2.11) describes. Indeed, the specification of the Hilbert space that one is working with is nothing but the mathematical counterpart to the specification of the system at hand. Accordingly, in (2.11), the system in the middle is not 'a message in the possession of Alice and Bob' (which would correspond to the Hilbert space $\widetilde{\mathcal{H}}_{AB}$), but 'a vacuum or message in the possession of Alice, and a vacuum or message in the possession or Bob', corresponding to $\mathcal{H}_A \otimes \mathcal{H}_B$.

Studying our scenario by resorting to this other system is unwieldy and clouds intuition. For instance, suppose we started the protocol with a completely mixed

state of the system. Then (assuming the operations $\mathcal{A}$ and $\mathcal{B}$ do not create any purity), following (2.11) will have us observe the system suddenly becoming partially pure, before returning to a completely mixed state. But this observation is a fallacy: our system never actually gained any purity. What happened, rather, is that the use of quantum circuits forced us to temporarily include into our description another variable, that of 'how many messages there are',[11] and to take into account that this variable has a definite state. Nevertheless, this piece of data is in fact *not* a variable, it is on the contrary an invariant assumption of our scenario – namely, that we are only dealing with one message. This sleight of hand between invariants and pseudo-variables is what leads to the temporary appearance of purity.

This becomes crucial, for instance, when studying the communicational properties of this scenario, as in Ref. [56]. In such a context, what we want to track is how the informational content of our precise system fares through the protocol; for instance, how different choices of $\mathcal{A}$ and $\mathcal{B}$ affect it. In the representation (2.11), our understanding of the communication capacity of these channels will be clouded by the fact that this communication capacity will take into account the fact that they preserve the number of messages – while this is irrelevant for our purposes, as this number of messages is not supposed to be a variable to transmit anyway.

The consequences of losing unitarity

A particular case of interest is that of the unitary version of this protocol. If we restrict to the scenario where $\mathcal{A}$ and $\mathcal{B}$ are unitary channels, then a description in standard quantum circuits has to use the non-unitary channels $\mathcal{E}$ and $\mathcal{D}$, even though the scenario itself is then fully unitary.[12] In other words, we get an example of a fully unitary scenario that cannot be described in unitary quantum circuits.

This is problematic as unitary evolutions and unitary scenarios feature important structure, that is lost without good cause in the standard description.[13] A typical example is reversibility: because $\mathcal{D}$ and $\mathcal{E}$ are not reversible, nothing in (2.11) allows us to say that the scenario is reversible when $\mathcal{A}$ and $\mathcal{B}$ are unitary, even though it is the case.

Another important property of unitary scenarios lies in their causal structure. Indeed, one remarkable feature of unitary channels is that they respect *causal atomicity* [69]:[14] if one input A of a unitary channel does not influence outputs B and C individually, then it does not influence the joint output BC either. Atomicity is critical to

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[11]To be fully precise, the extra variable can be understood as capturing the possible answers to the question 'are there zero messages, or one message shared between Alice and Bob, or two messages of which one is in the possession of Alice and the other in the possession of Bob'.

[12]Note that $\mathcal{E}$ can at least be said to be an isometric channel, but for $\mathcal{D}$ even this feature cannot be kept.

[13]This ties in directly with the previous point: this important structure derives from the conservation of information in unitary scenarios, a conservation that the standard description loses track of, because of the introduction of pseudo variables.

[14]The term 'causal atomicity' is not used in Ref. [69], even though the notion is introduced there (see Remark 4.4). The name was coined later in Refs. [4, 5].

our ability to define a sound notion of the causal structure of a unitary channel, in particular because it allows us to represent this causal structure as a a set of arrows between inputs and outputs – while in its absence one would also have to specify influence from each input to all possible combinations of outputs, something much less insightful and compelling. Beyond channels, these considerations straightforwardly extend to the definition of the causal structure of unitary scenarios (see Ref. [69]).

That the standard description of our scenario is not explicitly a unitary one is thus an obstacle to the study of its causal structure. This is made even more problematic by the fact that this scenario has been used to provide a comparison with scenarios featuring exotic causal structure [46, 47], so investigating its own causal structure is an important issue.

In fact, a recent paper building on the ideas of the present thesis showed that taking sectorial correlations and constraints into account allows one, not only to recover a good notion of causal structure (satisfying causal atomicity in particular), but even to refine it into a more detailed one [5] (see a summary in Section 6.3.2). This vindicates in hindsight the idea that there is much to be gained, in terms of causal analysis, in adopting a more refined perspective than the standard one.

Missing subsystems

We call $S = M \otimes C$ the global system that is being evolved in this scenario. A natural way to see the channels $\mathcal{A}$ and $\mathcal{B}$ is as having access to *subsystems* of S. Indeed, each of these channels can always be embedded (by taking the other channel to be the identity in (2.11)) to give an action on S, that is unitary when the channel is unitary; and furthermore, these two actions commute. This corresponds to recent proposals for an operational definition of subsystems as corresponding to commuting subsets of the set of operations on the global system (see Ref. [70] and references therein).

(2.11), however, does not lead to a proper formal depiction of how A and B embed as subsystems of S, because it only characterises them as subsystems of $A \otimes B$, with $\mathcal{H}_A \otimes \mathcal{H}_B \ncong \mathcal{H}_S$. Thus, as subsystems of S, the formalisation leaves it unclear how exactly they relate to each other, in which sense they transform it, and why such subsystems – not describable by tensor factors – are describable.

Yet mathematically, the situation is very well understood: such subsystems correspond to sub-C* algebras[15] (i.e. subalgebras that are closed under the adjoint) of $\mathrm{Lin}(\mathcal{H}_S)$ that are not factors. The idea that subsystems are described in the abstract by sub-C* algebras is a well-known one: it is a central tenet of algebraic quantum field theory [71], and has been argued for in quantum information on the grounds of both the structure of observables [72, 73] and that of dynamical transformations [70]. In finite dimension, a sub-C* algebra $\mathscr{A}$ of $\mathrm{Lin}(\mathcal{H}_S)$ can correspond to the space of operators of the form $M_A \otimes I_B$ in a factorisation $\mathcal{H}_S = \mathcal{H}_A \otimes \mathcal{H}_B$ – in which case

---

[15]Or equivalently, sub-von Neumann algebras: in finite dimension (to which we restrict ourselves here), the two notions coincide.

it is called a *factor* algebra –, but not only. The general case [70] is that the Hilbert space decomposes as

$$\mathcal{H}_S = \bigoplus_k \mathcal{H}_A^k \otimes \mathcal{H}_B^k, \tag{2.12}$$

and that $\mathscr{A}$ is the space of operators of the form $\bigoplus_k M_{A^k}^k \otimes I_{B^k}$. The space of operators of the symmetric form $\bigoplus_k I_{A^k} \otimes N_{B^k}^k$ is then the *commutant* of $\mathscr{A}$, i.e. the space of operators that commute with all operators of $\mathscr{A}$. The commutant of $\mathscr{A}$ can be thought of as defining the subsystem complementary to A within S [70].

We see that, up to a relabelling of the sectors, (2.10) is an instance of (2.12), with the sectorial constraints precisely enforcing the above form for operators: our physical intuition that A and B define subsystems of S checks the mathematical definition of subsystems as sub-C* algebras. It is thus unsatisfactory that this crisp mathematical underpinning of our notion of a subsystem finds no formal counterpart in the standard circuit framework. One can see that, generically, any subsystem corresponding to a non-factor sub-C* algebra will not be properly representable in this framework.

2.3 Causal decompositions of unitary channels

Another major part of this thesis' background is the study of causal decompositions [55, 69, 74, 75], which aims at exploring the connection between the *causal structure* and the *compositional structure* of unitary channels. As we will see, to unravel this connection, one is forced to go beyond standard quantum circuits, for reasons that are closely analogous to the ones exposed in the previous section.

2.3.1 A tentative equivalence between causal and compositional structures

Let us start with the notion of causal and compositional structures. Given a unitary channel with several inputs and several outputs (i.e., such that their input and output Hilbert spaces have preferred factorisations into tensor products), its causal structure is described by a set of no-influence relations. A no-influence relation is the fact that modifications of a given input cannot affect a given output. Formally, it is defined in the following way: if $\mathcal{U}$ is a unitary channel from inputs A and B to outputs C and D, one says that A cannot influence D (written $A \nrightarrow D$) if there exists a channel $\mathcal{C}$ such that

$$\tag{2.13}$$

where the symbol $\overline{\overline{\top}}$ denotes the trace-out channel.

Compositional structure, on the other hand, corresponds to the existence of decompositions of a given unitary channel into several unitary channels along a given graph. For example, there exist unitary channels from inputs A and B to outputs C and D that admit a decomposition of the following form:

$$
\begin{array}{c}
\mathcal{U}
\end{array}
=
\begin{array}{c}
\mathcal{U}_2 \\
\mathcal{U}_1
\end{array}
. \tag{2.14}
$$

Clearly, for a given unitary channel, the existence of a decomposition of the form (2.14) implies that this channel satisfies the no-influence relation $A \not\rightarrow D$, as described in (2.13). Interestingly, the converse is also true [76]: if a unitary channel satisfies $A \not\rightarrow D$, then it admits a decomposition of the form (2.14). The central conjecture that the research programme of *causal decompositions* aims to probe is that this equivalence between causal and compositional structures for unitary channels, which we just illustrated in a simple example, holds in general: for any number of inputs and outputs, a given set of no-influence relations is equivalent to the existence of a decomposition along a given graph, in which these no-influence relations are made obvious.

Proving this conjecture would unlock a remarkable correspondence between the causal properties of processes and their mathematical form: this could yield significant insight into the structural implications of causal structure, of both practical and fundamental value. So far, no counter-example to this conjecture has been found, and it has been proven in numerous cases; yet, in some of these cases, the compositional structure had to be expressed by going beyond standard quantum circuits.

2.3.2   Index-matching quantum circuits

The paradigmatic example of this is the case of unitary channels with three inputs A_I, E_I, B_I and three outputs A_O, E_O, B_O, obeying the no-influence relations $A_I \not\rightarrow B_O$ and $B_I \not\rightarrow A_O$. The causal decomposition corresponding to this pair of no-influence relations should have the following graph:

$$ (2.15) $$

However, if we take this graph to represent a standard unitary quantum circuit (i.e. if we interpret each box as a unitary channel), it is not equivalent to the causal structure: there exist unitary channels that obey the two previously mentioned no-influence relations, yet cannot be decomposed in the form of (2.15) (see Ref. [55] for an example). Yet there exists a slightly different kind of circuit for which the theorem holds [55], namely:

$$ (2.16) $$

The decomposition on the right-hand side is written in terms of *index-matching quantum circuits*, with distinctive 'k' superscripts written on some of the wires. Such diagrams were first introduced in Ref. [55], where they were called 'extended circuit diagrams'. In this thesis, we shall adopt the more specific name 'index-matching quantum circuits', and use somewhat different notation to that in the original work [55].[16] The superscripts can be interpreted in the following way (where this is again slightly different from the presentation in Ref. [55]). There exists a finite set of index values K; the Hilbert space $\mathcal{H}_R$ admits a partition into orthogonal subspaces $\mathcal{H}_R^k$, with $k \in K$; so do the other wires with 'k' superscripts. U_3 is a unitary map from $\mathcal{H}_R \otimes \mathcal{H}_{B_I}$ to $\mathcal{H}_{R'} \otimes \mathcal{H}_{B_O}$, that satisfies the additional requirement that it preserves each of the sectors, in the sense that for any k, one has $U_3(\mathcal{H}_R^k \otimes \mathcal{H}_{B_I}) = \mathcal{H}_{R'}^k \otimes \mathcal{H}_{B_O}$; a similar condition holds for U_2 (to put it in simple terms, U_2 and U_3 are block-diagonal). The combination of the wires L^k and R^k is the Hilbert space

---

[16]In comparison with Ref. [55], we drop the practice of writing superscripts in boxes, writing them only on the wires. Our presentation will also not include 'nested indices', i.e. superscripts of the form kl_k, because such nested indices are unnecessary for our needs.

$\bigoplus_{k \in K} \mathcal{H}_L^k \otimes \mathcal{H}_R^k$, and not $\mathcal{H}_L \otimes \mathcal{H}_R = \left(\bigoplus_{k \in K} \mathcal{H}_L^k \right) \otimes \left(\bigoplus_{l \in K} \mathcal{H}_R^l \right)$ as would be the case in an interpretation in standard circuits; so that U_1, for instance, is a unitary map to the former and not the latter. Similarly, L' and R' combine into $\bigoplus_{k \in K} \mathcal{H}_{L'}^k \otimes \mathcal{H}_{R'}^k$.

Any unitary satisfying $A_I \not\rightarrow B_O$ and $B_I \not\rightarrow A_O$ admits a decomposition of the form (2.16) [55]. It is therefore natural to argue that index-matching quantum circuits are the proper tool to study causal decompositions. Indeed, beyond this paradigmatic example, several other cases of causal decompositions have been proven which involve index-matching quantum circuits, and do not hold if one limits oneself to standard quantum circuits (see Ref. [55] for an overview); it is reasonable to expect that, if the conjecture were to be proven true, any sufficiently complex causal decomposition would generically involve index-matching.

We can see that the features that differentiate index-matching quantum circuits from standard ones are precisely the ones we already encountered in Section 2.2.1, namely, sectorial constraints on evolutions, and sectorial correlations defining non-standard parallel compositions, with the two playing together in a precise way so as to preserve consistency. It is remarkable that two starkly different lines of inquiry – one stemming from physical and conceptual considerations, and the other from mathematical and formal ones – led to the discovery of the same structure; this provides a further clue to the fundamental importance of that structure for the study of quantum theory.

In fact, further analysis reveals that the roots of the standard description's inadequacy in this context are very close to the ones that we expounded upon in Section 2.2.2 in the context of superpositions of trajectories. In particular, the necessity to explicitly preserve unitarity plays a crucial role here. A deeper connection is that the structural root of the need for indices in causal decompositions lays in the general form (2.12) of sub-C* algebras.[17]

The literature on causal decompositions does not only strengthen our understanding of the problem with standard quantum circuits: it also introduces us to a commencement of a solution, in the form of index-matching quantum circuits, in which sectorial constraints and correlations are explicitly depicted. However, before the present thesis, such circuits were only used in a makeshift way, with their meaning defined by hand in simple cases: there was no theory of the mathematical framework that they represent. The theory of routed quantum circuits, introduced in Chapter 3 of this thesis, aims to draw on the intuition provided by index-matching quantum circuits in order to build such a general and consistent framework, that would also capture all situations of the form of the one described in Section 2.2.

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[17]This can be seen in the genealogy of the proof of the causal decomposition (2.16) in Ref. [55]: it uses a theorem proven in Ref. [74], which itself relies on a theorem of Ref. [77], originally proven constructively in Ref. [78], but for which Ref. [77] provides a simple proof relying on the theory of C* algebras. In unpublished work, we bypassed this and showed that all of the causal decompositions presented in Ref. [55] could be proven in an elegant and concise way by using elementary considerations on C* algebras, so that one can immediately observe how the general form of the latter leads to the introduction of indices in causal decompositions. Interested readers are encouraged to contact us (i.e. me) for further information.

In a nice throwback, Section 3.4 will then show how index-matching quantum circuits themselves can be seen as a handy diagrammatic representation of a sub-framework of routed maps: the framework of *index-matching routed maps*. This will allow us to properly formalise such diagrams in full generality, to provide them with rigorous semantics, and to prove that simple rules single out the physically meaningful index-matching quantum circuits, such as (2.16).

2.4 Indefinite Causal Order

Before we get there, we introduce another line of research that challenges the standard framework of quantum circuits, that of *indefinite causal order* (ICO). This time, the deviation from quantum circuits will not lay in the presence of sectorial constraints and correlations, as in Sections 2.2 and 2.3, but in the existence of a cyclic ordering of operations. Despite this, a remarkable result of Chapter 5 will be that there are in fact deep links between these two departures from standard circuits: sectorial constraints and correlations can be used to display intuitively, and check easily the consistency of, the allowed cyclic compositional structures.

ICO has received considerable attention from the quantum foundations community, for more than a decade now. Following the seminal papers [16–18],[18] many aspects of it have come under study: its physicality, its certification, its purported implementations as well as the precise physical meaning of these implementations, the advantages that its use would yield over causally ordered quantum scenarios in communication, computation and thermodynamics, its formal aspects, and many others. Here, keeping with the ambition of this thesis, we will leave a lot of these aspects aside, and focus on the challenges that ICO poses to the circuit framework. As we explain in Section 2.4.3, we hope that the work carried out on this front in this thesis can spark progress on the other topics of enquiry by making the mathematical handling and invention of exotic processes more intuitive.

2.4.1 The supermaps framework

The best starting point to reach ICO is the framework of supermaps.[19] The original idea is to restate the quantum circuit framework presented in Section 2.1 in a different way, by focusing on the circuit architectures themselves, rather than on the operations. Roughly speaking, a circuit architecture is 'a circuit with holes', with the holes standing in for yet-unspecified operations: the circuit architecture defines how these operations are connected together. This naturally takes the form of a theory of

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[18]See also Ref. [79] for a conceptual precursor.

[19]Another equivalent framework, that of *process matrices* [18, 59], is also in use in the ICO literature. Process matrices are just the Choi-Jamiołkowski representation of supermaps: using them allows one to compute outcome probabilities in a more direct way in an operational picture, but this comes at the price of clouding the nice conceptual intuitions about higher-order processes as simply mapping channels to channels. We expand on the conceptual and mathematical relationship between the two formalisms in Appendix C.1.
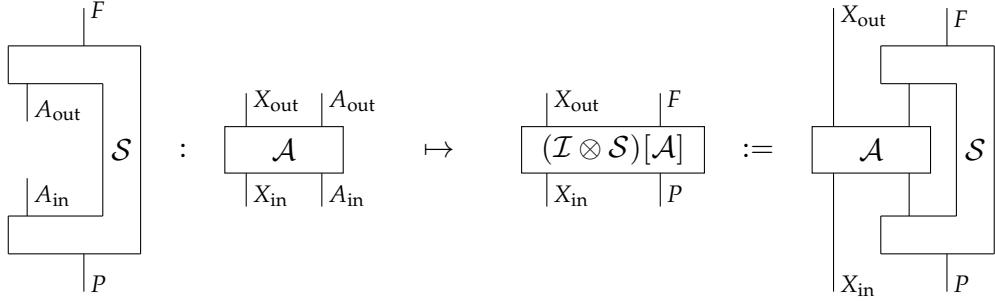
FIGURE 2.1: Diagrammatic representation of a superchannel $\mathcal{S}$, and
of its action on a channel $\mathcal{A}$ (that also acts on an auxiliary system),
yielding a channel $(\mathcal{I} \otimes \mathcal{S})[\mathcal{A}]$.

higher-order processes: the global circuit architecture is represented by a superchannel,
a mathematical object that takes in channels (representing the choice of the operation
plugged in each hole) and yields a channel (representing the global channel obtained
by connecting them in the manner stipulated by the superchannel).[20]

It is instructive to draw a parallel with the way in which quantum channels act
on quantum states. Indeed, quantum channels can be defined as the only mappings

$$\mathcal{C} \in \mathrm{Lin}\left[\mathrm{Lin}(\mathcal{H}_A^{\mathrm{in}}) \to \mathrm{Lin}(\mathcal{H}_A^{\mathrm{out}})\right] \tag{2.17}$$

that preserve all quantum states (i.e. positive and trace-one matrices), including
quantum states on an extended system $\rho \in \mathrm{Lin}[\mathcal{H}_A^{\mathrm{in}} \otimes \mathcal{H}_X]$. In other words, the
condition on $\mathcal{C}$ is

$$\forall X, \, \forall \rho \in \mathrm{Lin}[\mathcal{H}_A^{\mathrm{in}} \otimes \mathcal{H}_X],$$
$$\rho \text{ is a quantum state} \implies (\mathcal{C} \otimes \mathcal{I})(\rho) \text{ is a quantum state.} \tag{2.18}$$

Similarly, considering first monopartite superchannels – i.e. superchannels acting
on a single operation –, we can define them [15] as the linear mappings

$$\mathcal{S} \in \mathrm{Lin}\left[\mathrm{Lin}\left[\mathrm{Lin}(\mathcal{H}_A^{\mathrm{in}}) \to \mathrm{Lin}(\mathcal{H}_A^{\mathrm{out}})\right] \to \mathrm{Lin}\left[\mathrm{Lin}(\mathcal{H}_P) \to \mathrm{Lin}(\mathcal{H}_F)\right]\right] \tag{2.19}$$

that preserve all quantum channels – including quantum channels on an extended
system $\mathcal{A} \in \mathrm{Lin}\left[\mathrm{Lin}(\mathcal{H}_A^{\mathrm{in}} \otimes \mathcal{H}_X^{\mathrm{in}}) \to \mathrm{Lin}(\mathcal{H}_A^{\mathrm{out}} \otimes \mathcal{H}_X^{\mathrm{out}})\right]$. In other words, the condition is

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[20]In this thesis, we will use the word 'supermap' for a generic higher-order map, that need not map
channels to channels, and call 'superchannels' the ones that do preserve trace-preservingness. In other
words, superchannels are to supermaps what CPTP maps are to CP maps. This is in contrast with the
terminology of Ref. [25], in which 'deterministic supermaps' correspond to what we call superchannels
here.

$$\forall X_{\text{in}}, X_{\text{out}}, \ \forall \mathcal{A} \in \text{Lin}\left[\text{Lin}(\mathcal{H}_A^{\text{in}} \otimes \mathcal{H}_X^{\text{in}}) \to \text{Lin}(\mathcal{H}_A^{\text{out}} \otimes \mathcal{H}_X^{\text{out}})\right],$$

$$\mathcal{A} \text{ is a quantum channel} \implies (\mathcal{S} \otimes \mathcal{I})(\mathcal{A}) \text{ is a quantum channel.} \quad (2.20)$$

The action of such an $\mathcal{S}$ is represented diagrammatically in Figure 2.1.

Note how this definition does not rely on any assumption about the circuit structure described by $\mathcal{S}$. (2.20) is a minimal, purely logical requirement: whatever $\mathcal{S}$ is, its action does not map us outside of quantum theory.[21] Yet it has been proven [15] that all monopartite superchannels have the form of a pre- and post- processing of their input channel, i.e. the form

$$(2.21)$$
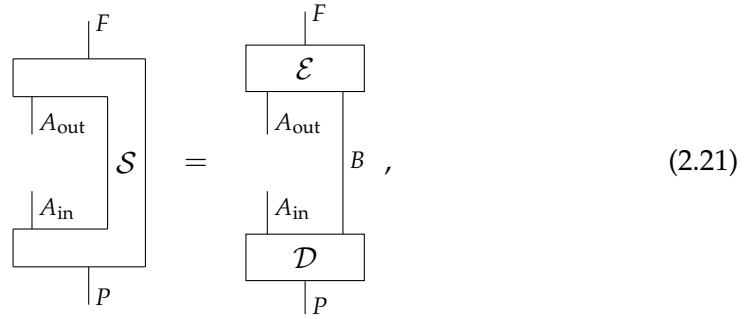
where $\mathcal{D}$ and $\mathcal{E}$ are quantum channels. We see that this superchannel is obviously implementable, as it just consists in nesting the input operation between two other channels. This vindicates in hindsight our choice of a minimal definition of monopartite superchannels: that definition is sufficient to narrow the range of superchannels down to the natural scenarios. It is for multipartite superchannels that the situation gets more interesting.

Indeed, we can now extend this definition to superchannels that act on several channels – i.e. 'circuits with several holes'. Let us present the case of bipartite superchannels, acting on pairs of channels; the generalisation to n parties is immediate.[22]

A bipartite superchannel is defined [17] as acting on a pair of channels, each possibly acting on an ancilla – i.e. on $\mathcal{A} \in \text{Lin}\left[\text{Lin}(\mathcal{H}_A^{\text{in}} \otimes \mathcal{H}_X^{\text{in}}) \to \text{Lin}(\mathcal{H}_A^{\text{out}} \otimes \mathcal{H}_X^{\text{out}})\right]$ and $\mathcal{B} \in \text{Lin}\left[\text{Lin}(\mathcal{H}_B^{\text{in}} \otimes \mathcal{H}_Y^{\text{in}}) \to \text{Lin}(\mathcal{H}_B^{\text{out}} \otimes \mathcal{H}_Y^{\text{out}})\right]$ – and returning a channel.[23] The diagrammatic representation of this action is represented on Figure 2.2.

Once again, we picked a minimal definition, merely asking for logical consistency. What range of situations does it allow for? From the results of Section 2.1, we

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[21]There is also a requirement of linearity of $\mathcal{S}$, which is usually motivated by the preservation of classical mixtures, although one can also do away with it and recover it from basic locality assumptions [80].

[22]Note that the construction presented here can be cast in a neater, categorical way, which also allows one to naturally extend it to the case of infinite-dimensional systems [80, 81].

[23]More precisely, bipartite superchannels were originally defined as acting on the larger space of all non-signalling channels on the tensor product of their two slots, i.e. on channels from $A_{\text{in}} \otimes X_{\text{in}} \otimes B_{\text{in}} \otimes Y_{\text{in}}$ to $A_{\text{out}} \otimes X_{\text{out}} \otimes B_{\text{out}} \otimes Y_{\text{out}}$ that are non-signalling from $A_{\text{in}}X_{\text{in}}$ to $B_{\text{out}}Y_{\text{out}}$ and from $B_{\text{in}}Y_{\text{in}}$ to $A_{\text{out}}X_{\text{out}}$. ('Non-signalling' is defined here through an analogue to (2.13).) However, it was proven at the same time that the well-defined superchannels on pairs of channels are exactly the same ones as superchannels on non-signalling channels, so we can overlook this difference.
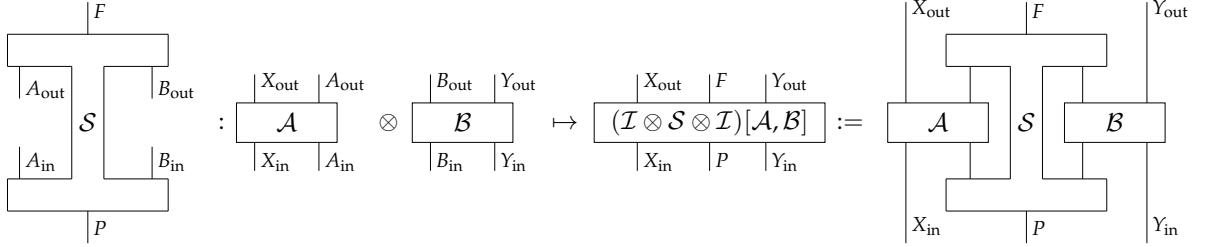
FIGURE 2.2: Diagrammatic representation of a superchannel $\mathcal{S}$ acting on a pair of channels $\mathcal{A}$ and $\mathcal{B}$ (also acting on auxiliary systems), yielding a channel $(\mathcal{I} \otimes \mathcal{S} \otimes \mathcal{I})[\mathcal{A}, \mathcal{B}]$.
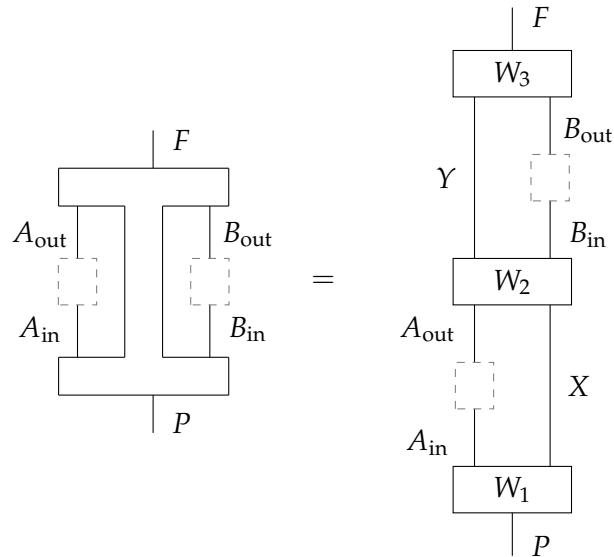
FIGURE 2.3: An example of a quantum comb, i.e. a superchannel with a definite causal order [10]. In this example, the $A_{\text{in}} \rightarrow A_{\text{out}}$ operation is applied before the $B_{\text{in}} \rightarrow B_{\text{out}}$ operation.
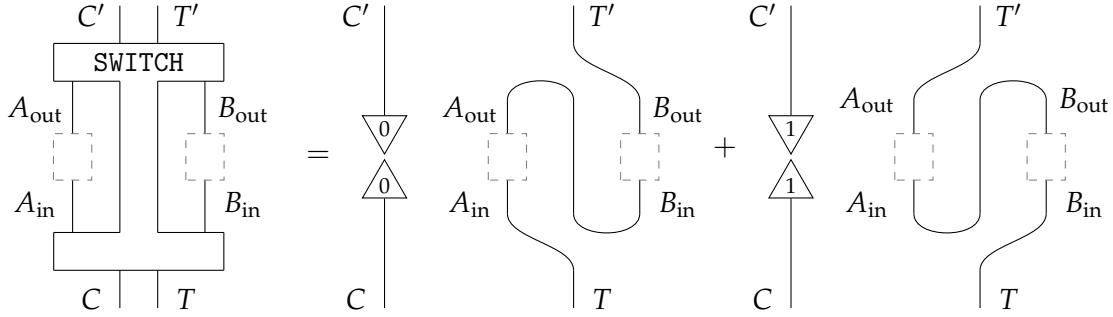
FIGURE 2.4: Circuit decomposition of the switch. The left term in the sum projects onto the $|0\rangle$ state of the control and implements Alice's transformation before Bob's. The right term has a similar interpretation. Formally, as noted in Section 2.1, the wire bent into a 'U' shape can be interpreted as the unnormalised Bell ket $|00\rangle + |11\rangle$, and the upside-down 'U' as the corresponding bra.
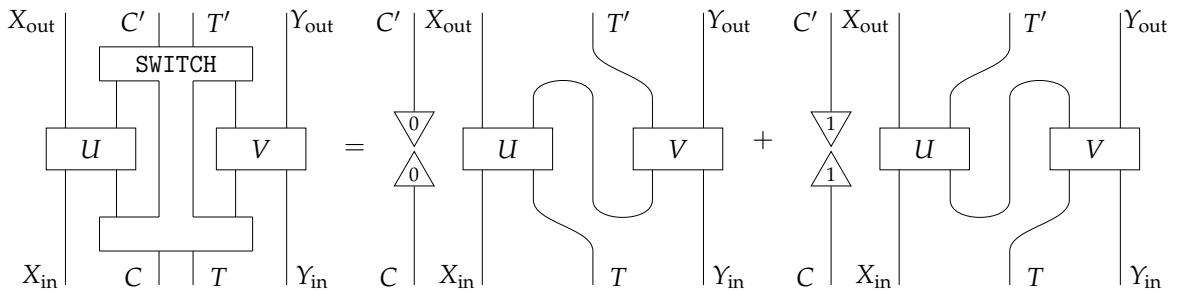
FIGURE 2.5: The action of the switch on a pair of unitary operators. The order of implementation of unitaries on the target system and ancillas is coherently controlled.

know that all superchannels in which the different input operations are arranged in a non-cyclic manner, possibly interspersed with intermediary channels, define valid superchannels. Such superchannels are characterised as *quantum combs* [10] (see Figure 2.3 for an example). But there are others: it is this realisation that kickstarted the study of indefinite causal order.

2.4.2 Some exotic superchannels

Indeed, the main payoff of the seminal papers [16, 18] is to provide examples of multipartite superchannels that are not combs, i.e. that cannot be modelled as non-cyclic arrangements of their input operations. These examples turned out to be the two paradigmatic ones in the bipartite case: the quantum switch, and the OCB process.

The quantum switch [16, 17] can be summarised as an arrangement of channels $\mathcal{A}$ and $\mathcal{B}$ in which a qubit coherently controls whether $\mathcal{A}$ is applied before $\mathcal{B}$, or $\mathcal{B}$ is applied before $\mathcal{A}$. To simplify things, we will define it here in pure quantum theory, as a linear map that transforms linear operators on a Hilbert space to linear operators on a Hilbert space, as opposed to a map between completely positive operators.[24]

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[24]Generally speaking, there will be some amount of back and forth between pure and mixed superchannels in this thesis. We trust the reader to parse between these, in the same way that one can easily switch between pure and mixed quantum theory whenever needed.

The SWITCH supermap is represented in Figure 2.4. Given two input operators $U : \mathcal{H}_A^{\text{in}} \to \mathcal{H}_A^{\text{out}}$ and $V : \mathcal{H}_B^{\text{in}} \to \mathcal{H}_B^{\text{out}}$, where all the spaces have the same dimension d, SWITCH returns an operator acting on $\mathcal{H}_C \otimes \mathcal{H}_T$, where C and T have dimensions 2 and d respectively, of the form

$$\text{SWITCH}(U, V) = |0\rangle \langle 0| \otimes VU + |1\rangle \langle 1| \otimes UV. \qquad (2.22)$$

More generally, as we saw, U and V could be acting on their own local ancillary systems, X and Y respectively. SWITCH is defined as follows:

$$\text{SWITCH}(U, V) = |0\rangle \langle 0| \otimes (I_X \otimes V)(U \otimes I_Y) + |1\rangle \langle 1| \otimes (U \otimes I_Y)(I_X \otimes V). \qquad (2.23)$$

This action is represented in Figure 2.5. If U and V are both unitary operators, then one can directly see that $\text{SWITCH}(U, V)$ is also a unitary operator. We call superchannels like this, that always map unitary operators to unitary operators, *superunitaries*. A little reflection reveals that any superunitary uniquely defines a superchannel, i.e. a map on channels in the sense of Section 2.4.1, via the Stinespring dilation of the channels.

It is obvious by construction that the quantum switch is not a comb. We thus see that our minimal definition of multipartite superchannels admits exotic instances. This begs the question: are these instances physical? Much of the subsequent literature has focused on tackling this question in different ways – especially in the case of the switch –, leading to contrasted answers.

Besides the switch, another important example is the OCB process, introduced in the other seminal paper for the field, Ref. [18].[25] A remarkable feature of the OCB process is that in an operational picture, in which the two input operations are seen as describing the actions of some local agents Alice and Bob, who can use them to implement measurements and record outcomes, it yields outcome probabilities that violate so-called *causal inequalities*. Causal inequalities, also introduced in Ref. [18], are to causal order what Bell inequalities are to locality: their violation provides a device-independent characterisation of the fact that the correlations experienced by Alice and Bob cannot be explained by them being in a well-defined causal order, or even in a classical mixture of well-defined causal orders. Importantly, the switch cannot violate causal inequalities:[26] this means that the OCB process features a stronger form of indefinite causal order. Superchannels that violate a causal inequality are sometimes called *non-causal processes* [83].

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[25]Even though it is posterior to Ref. [16], which already presented an exotic process, and to Ref. [10] in which part of the mathematical framework was presented already, Ref. [18] can be credited with laying down solid conceptual bases for the operational interpretation of higher-order processes in potential theories of physics, where Ref. [16] (and its later, more refined version [17]) only presented them as computational tasks. In our view, Refs. [16, 18] should be seen on an equal footing as the two parents of the field.

[26]However, it was proven in a very recent paper [82] that the switch can violate a so-called *local-causal inequality*, in which the assumption of the existence of a well-defined causal order is supplemented with a (weak) locality assumption.

The quantum switch is the paradigmatic example of processes with coherent control of causal order, in which the order between parties (i.e. between input operations) is under the control of a quantum variable. Starting with three parties, this can be generalised to *dynamical* coherent control of causal order, in which any party is allowed to affect the order between subsequent parties. Processes that feature (possibly dynamical) coherent control of causal order have recently been characterised in general in a constructive way, under the name of *quantum circuits with quantum control* (QC-QCs) [84]. Different proposals for physical implementations of the switch – that can easily be extended to ways of implementing QC-QCs in general – have been proposed, and some of these proposals have been performed experimentally, prompting an ongoing debate as to what counts or would count as a genuine implementation of the switch. Importantly, QC-QCs cannot violate causal inequalities [84].

By contrast, in our knowledge, no proposal for a physical implementation of the OCB process has been put forward yet, be it in standard or in exotic physics. On the contrary, some effort has been undertaken to introduce physical principles that would restrict the set of admissible superchannels. An important such proposal is the principle of unitary extendibility [59].[27] Remember that we noted that the switch was a unitary superchannel, or superunitary, as it always mapped unitary input channels to a unitary output channel. As proven in Ref. [59], unitarity of a superchannel is equivalent to the unitarity of its CJ representation (i.e. its process matrix) seen as a channel.[28]

The principle then works in analogy to the Stinespring dilation, which tells us that any quantum channel can be extended to a unitary channel with a pure state fed into its ancillary input, and its ancillary output discarded. Similarly, the principle of unitary extendibility requires that a physical superchannel should be extendible to a unitary superchannel with a pure state fed into its ancillary input, and its ancillary output discarded. A possible motivation for upholding this principle is the belief in the fundamental reversibility of physical processes. This excludes the OCB process, whose Stinespring dilation features a unitary that does not define a valid superchannel [59].

One could hope that the principle of unitary extendibility would be sufficient to exclude processes that violate causal inequalities. This is indeed true in the bipartite case, as bipartite superunitaries can be proven to all be either causally ordered, or variations of the quantum switch [75, 85]. However, this intuition fails in general: there exist tripartite superunitaries that violate causal inequalities.

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[27]In Ref. [59], this is called the 'purification principle', but we prefer the term 'unitary extendibility', as 'purification' usually refers to purification to an isometry and not to a unitary, and any superchannel is trivially purifiable in that sense.

[28]More intuitively, this can also be characterised as the fact that the channel obtained by plugging swaps with ancillary systems into each slot of the superchannel is a unitary channel.

The paradigmatic example of this is the Lugano process [86, 87], an exotic tripartite process that was originally introduced as a *classical* superchannel,[29] and whose unitary extension to quantum theory can be derived in a straightforward way [59]. The Lugano process maximally violates some causal inequalities [86, 87]. It has no known physical implementation (except for a very recent proposal based on time-delocalised subsystems [51]). We leave the description of this process to Section 5.4.3, in which we propose an intuitive account that we hope will be more enlightening than its mathematical specification.

The discovery of the Lugano process leads to new questions. It shows that the principle of unitary extendibility fails to exclude processes that violate causal inequalities, so that an axiomatic approach would have to come up with other principles in order to leave these out. More interestingly, the fact that the Lugano process can also be presented as a classical superchannel seems to contradict the original belief that ICO is to be understood as a 'quantumness of causal relations': some instances do not seem to involve any kind of typically quantum behaviour. More precisely, causal inequality violations in the Lugano process can be obtained without ever resorting to incompatible experimental contexts. This makes a 'new physics' interpretation of the non-causal processes even more puzzling.

Adopting the superchannel framework led us to a particularly intriguing situation: a minimal definition, in which one merely asks for basic theoretical consistency, – one that worked fine, at the lower level, to single out quantum channels – leaves the door open for exotic scenarios, some of which admit more or less controversial physical interpretations, and some of which have remained completely cryptic so far yet haven't been properly eliminated on the ground of physical principles. In our view, a major cause of obscurity in that context is that even the logical structure of most processes remains impenetrable, due to the lack of a satisfactory circuit model to express it.

2.4.3   Why we need a circuit model

In keeping with this thesis' focus on expressive compositional techniques to capture quantum theory's structure, we will concentrate on this task: designing a suitable circuit model for ICO. Let us describe the current situation on this front and argue why progress in this direction would be highly beneficial.

We start with a contrasting situation. Causally ordered architectures of quantum circuits now admit a number of expressive and pliable frameworks, e.g. in terms of process theories or as quantum combs. These frameworks feature built-in consistency, introduce a steady conceptual and mathematical architecture for describing

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[29]In Ref. [86], it is presented as a 'classical process matrix', defined as a diagonal quantum process matrix. A more intuitive definition is to frame it as a higher-order classical process, defined in the same way as higher-order quantum processes were in Section 2.4.1: it takes classical channels (i.e. stochastic matrices) as input and maps them to a classical channel.

their objects, and usually work as a formal basis for insightful diagrammatic representations. All of these features in turn make the study of their objects considerably easier, faster, and more intuitive: the mathematical and conceptual architecture allows one to state and prove powerful and general theorems, clarifying further the properties of the objects; the built-in consistency and the accurate diagrammatic representations make their handling both safe and intuitive; finally, the generality of the framework opens the door for scaling up to more and more involved scenarios, including with numerical means.

In comparison with this, the available models for the manipulation of exotic processes are still rudimentary. The superchannel of a higher-order process is an undifferentiated blend of all of the causal influences involved, fused into a high-dimensional linear operator. Parsing its structure and behaviour is possible, at best, only through a careful inspection of it by a person sufficiently experienced with the quirks of the framework; no formal tools will be there to help.[30] This makes the handling of even relatively modest processes very time- and energy-consuming, while more involved processes (with higher dimensions, more parties, or more complex information processing between the parties) quickly become virtually impossible to consider in detail.

We believe that this situation is currently a major obstacle to achieving substantial progress in any of the areas of investigation on ICO. The study of the practical advantages that it confers will rely on little more than blind-guessing if one is not able to build a sound and nuanced intuition about the processes' behaviour; research about the general form of exotic processes will lack even the language to properly express that general form; thinking of ways of implementing a process will remain strenuous as long as one does not even have an insight of what the process does logically, etc. Moreover, in each of these research programmes, scaling up the intuitions painfully obtained on simple examples will be an uphill battle. Thus, progress in the expressiveness and user-friendliness of the framework will be a prerequisite to progress in other directions.

A striking manifestation of the difficulties entailed by the primitiveness of the bare superchannel framework is the fact that there are so few currently known exotic processes. The reasons are the same as the ones previously exposed: as building an exotic process constitutes a thin balancing act between introducing circularity of the causal influences and maintaining logical consistency, attempts at it will quickly become intractable in the absence of specific tools to support intuition about these moral principles. Moreover, the only available way to ensure that a process is a valid one is to check its consistency by hand – a brute-force, time-consuming endeavour. Finding ways to bypass this specific difficulty will be one of the main objectives of our Chapter 5.

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[30]The situation is even slightly worse when the process is presented as a process matrix, because the use of the CJ isomorphism flattens out the input/output distinctions within the superchannel; see Appendix C.1.

2.4.4   The existing frameworks for indefinite causal order

We are not the first to tackle these questions, and the recent years (in particular the same years during which this thesis itself was developed) have seen substantial progress on the design of more informative frameworks for the manipulation of higher-order processes. Here, we review them and comment on their strengths and weaknesses with respect to our own demands for a suitable circuit model.

The type structure of higher-order process theories

A first line of improvement has been the study of the *type structure* of higher-order process theories, i.e. of the language with which one can describe the structural role (type) of a higher-order process – e.g. what it acts on and what it yields. A particular outcome is the ability to compute the equivalence of different types, and to see these equivalences as a model of a certain logic. In turn, this allows one to express ways in which higher-order processes can be composed together to form other higher-order processes, and the rules that constrain the legal compositions. The upshot is that compositional frameworks of this kind thus allow one to safely build up compound processes from basic ones, in a modular way.

On this subject, Refs. [88, 89] provide a formal language to recursively build and classify the types of quantum higher-order processes. Ref. [90] presents a generic construction of higher-order process theories over sufficiently well-behaved base theories, using the language of category theory, and characterises these higher-order theories as *-autonomous categories, whose types are a model of multiplicative linear logic. Ref. [91] further shows that taking additional structure of the base theories into consideration leads to a more refined type system for the higher-order theories, that forms a model of BV logic. Ref. [92] specifically considers the problem of the admissible compositions of higher-order processes, and Ref. [93] focuses on the characterisation of higher-order types using linear projectors. A parallel line of research [94, 95] derives similar results by characterising the structures of higher-order frameworks in their own right, without referring to their construction from a base theory.

While this represents considerable progress, we believe that these frameworks are still not sufficiently fine-grained to provide a suitable understanding of exotic processes. In particular, it is unlikely that these type systems are expressive enough to certify the validity of a modular construction of these exotic processes. For example, while these frameworks characterise the types of, say, the switch or the Lugano process, and the ways to compose them into bigger processes, they do not offer a presentation of the way in which they are themselves built – i.e. of the way in which they connect the operations on which they act. In other words, exotic processes are still introduced as basic bricks, that cannot be broken down further. Understanding their inner mechanics would require to move to a more refined picture.

Diagrammatic calculi

Work has also been undertaken to develop frameworks for quantum control and indefinite causal order from a more Computer Science-like perspective, focusing in particular on the design of diagrammatic calculi, that would support the intuitive manipulation of quantum control architectures at the graphical level. It is noteworthy that these endeavours have generically led to frameworks that capture both quantum control, such as superpositions of trajectories as described in Section 2.2, and indefinite causal order: the same will happen in this thesis, in which routed circuits will be used to describe both. Note that the shortcomings of these frameworks with respect to our own goals, as described below in the context of indefinite causal order, apply to the case of standard quantum control as well.

A first recently developed approach is that of PBS calculus [96, 97] (see also the similar LOv calculus [98], which however does not aim at capturing indefinite causal order). The PBS calculus is primarily aimed at describing quantum-optical architectures and the form of quantum control that they allow for, in particular through the use of polarising beam splitters (PBS). It offers an equational theory through which the equivalence between two such architectures can be checked for equivalence. PBS calculus provides a firm formal axiomatisation of optical diagrams and can be applied, in particular, to resource minimisation in photonic quantum computing [99]. Its pure version has semantics in term of unitary gates;[31] thus any PBS diagram with holes seems to define a superunitary (see below on this), so that PBS diagrams can contribute to the design of sound methods for building consistent processes with indefinite causal order.

An important divergence with respect to our own goals is that the parallel composition in PBS diagrams corresponds to the direct sum, not to the tensor product; this makes their interpretation starkly different.[32] In particular, it makes the problem of whether they define valid superunitaries more subtle than one might have thought at first glance. Indeed, superchannels are required to be well-behaved also when acting on ancillary systems; but the integration of such ancillary systems into a PBS diagram is not a straightforward procedure, as they are in a tensor product with other systems. Note that extending PBS calculus to noisy quantum theory requires to consider not quantum channels, but choices of purifications of them [97], which makes the formalism unwieldy in this case.[33] It is also unclear how flexibly PBS diagrams can be used to model architectures beyond the optical ones, and whether they

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[31]See Proposition 10 in Ref. [96].

[32]For some linear-optical computations, one can circumvent this discrepancy by using an exponentiation functor that maps from the description of a single particle's degree of freedom to the Fock space description of an unknown number of such particles [100]. This functor maps the direct sum to the tensor product. However, it does not preserve the trace – in fact, there is not even a trace structure on Fock spaces as their dimension is infinite. This means that exponentiation won't work in the cases involving feedback loops, which are precisely the ones we are interested in here.

[33]This can be understood as a consequence of the impossibility of defining a superchannel for quantum control; we will discuss this problem in depth in Chapter 4. In this chapter, we will argue that it is more accurate to consider quantum control as performed on sector-preserving channels acting on a $d + 1$-dimensional system, rather than as acting on a d-dimensional system as done in Refs. [47, 97],

can describe more exotic processes such as the Lugano process.

The framework of *addressable quantum gates* [101] also aims at capturing processes featuring indefinite causal order in a way that makes their layout explicit. It does so by explicitly soft-coding the wiring between gates into address registers that the gates themselves can access. However, addressable quantum circuits do not define a superchannel, but rather an infinite sequence of unitary evolutions, with some of them possibly put into loops (meaning, in this context, that they get applied over and over again to the target system). Even though the switch for example can be obtained by taking a particular such sequence and halting it at a specific step, it is unclear in which formal way, and under which conditions, a generic addressable quantum circuit can be used to define a valid superchannel.

A recently developed graphical language, the many-worlds calculus [102], aims at formally capturing quantum control by describing both monoidal structures of linear maps – the tensor product and the direct sum – at once. This yields an intuitive diagrammatic representation of the switch. However, this diagrammatic representation cannot be used to certify that the switch is a valid superchannel, as the semantics of many-worlds calculus is in linear maps, not in the sub-theory of the isometric or unitary ones. It is also unclear whether this calculus can be extended to the case of noisy quantum channels (represented as completely positive maps), and whether it can be used to intuitively represent more involved cases of indefinite causal order, such as dynamical coherent control or the Lugano process.

Quantum circuits with quantum control

We end this review with a particularly important development with respect to our goals: the introduction of the class of *quantum circuits with quantum control* (QC-QCs) [84]. Members of this class are the superchannels featuring (possibly dynamical) coherent control of causal order – in fact, QC-QCs can be seen as formally defining what it means for a superchannel to feature this form of indefinite causal order.

Ref. [84] describes a constructive way of building up the class of QC-QCs, in a bottom-up approach; furthermore, this constructive method yields some intuition as to the structure of the superchannels, as the basic building blocks describe how some systems are used to coherently control the order of application of channels. It thus partly meets our demand for an intuitive circuit model in which the consistency of superchannels would be ensured, and through which their compositional structure would become transparent.

However, by construction, QC-QCs only describe dynamical coherent control of causal order, which represents a 'weak' form of indefinite causal order: in particular, as proven in Ref. [84], QC-QCs cannot violate causal inequalities. This thus leaves aside more exotic processes such as the Lugano process, even though these are the

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precisely because the latter option forces one to distinguish between different possible implementations of the channel.

ones for which obtaining an intuitive presentation would be the most beneficial, given their cryptic features.

Moreover, even though Ref. [84] adopts a constructive approach, it puts little emphasis on the connectivity of the processes it describes: in particular, it offers no diagrammatic representation of their compositional structure. More precisely, the figures presented in Ref. [84] represent each input channel as delocalised, with its application under the control of other systems; this allows to represent the process without using feedback loops, but comes at the price of not representing clearly the superchannel itself, which should be acting on each input channel separately. In particular, this makes the presentation awkward in the case in which the input channels are also acting on ancillary systems.

2.5 Conclusion

In this chapter, we presented the framework of quantum circuits then introduced several recent developments in the study of quantum theory that call for the development of extensions to this framework. Loosely speaking, their common point is the appearance, in one form or another, of *coherent control* (or quantum control):

- coherent control of the application or not of a gate in Section 2.2;

- coherent control of which causal decomposition gets instantiated in Section 2.3;

- coherent control of the causal order in which operations are applied in Section 2.4.

In each case, we argued in detail why these forms of coherent control could not be captured by standard quantum circuits. Given the ubiquitous nature of coherent control, we expect that future developments on both the fundamental and the applied aspects of quantum theory will keep digging out other instances, each posing a further challenge to the standard circuit model. There is thus a pressing need for the introduction of a more general model, able to capture coherent control in its most general form.

We believe that the framework of routed circuits, introduced in this thesis, can be this model, or at least constitute one of its core components. Routed circuits will not present themselves as a fine-grained theory, allowing to describe protocols in great detail and derive a lot of results; in particular they will yield no diagrammatic calculus, at least no more than standard circuits or string diagrams do. On the contrary, the goal pursued here is to be *as minimalist as possible*: to pin down precisely the crucial features that are necessary to make the representation meaningful, and nothing else. The hope is that this minimalism will imply generality, i.e. that all the different forms of coherent control will be amenable within this framework. Over

this minimal backdrop, it will then be possible to add more descriptive overlays, suitable to one's needs.

Chapter 3

Routed circuits

But the Greeks, our masters, knew well that Aphrodite is not born of a natural fertilisation; beauty will never be a natural production; it can be obtained only through an artificial constraint.

André Gide, *New Pretexts*.

In this chapter, we display a minimal extension to the standard quantum circuit framework that captures scenarios with coherent control, in the absence of indefinite causal order (which will be treated in Chapter 5). In particular, our goalpost will be to obtain a satisfactory formalisation of the paradigmatic examples discussed in Chapter 2: superpositions of trajectories (Section 2.2) and index-matching causal decompositions (Section 2.3).

It is important to spell out precisely what we mean by a 'satisfactory' formalisation here. A first minimal requirement for us is that our framework should form a *circuit theory*, in the sense of Section 2.1.1: it should feature notions of sequential and parallel compositions, allowing one to safely build non-cyclic circuits in an incremental way, and to provide sound diagrammatic intuition. We would also like these diagrams to be as expressive as possible of the supplementary structure of the new framework. In line with our comments on the unsatisfactory aspects of standard circuits for the formalisation of the scenarios at hand, the framework should describe accurately the Hilbert spaces in use in the case of non-standard parallel composition. Finally, it should carry structural theorems determining whether the physicality of the evolutions (i.e. isometricity, unitarity, or trace-preservingness, depending on the case) is maintained.[1]

---

[1]Note that this represents a departure from circuit theories in the case of the theory's restriction to physical maps. In standard circuits, the latter form a circuit theory as well, as discussed in Section 2.1.2. In routed circuits, while routed *linear maps* form a circuit theory, routed *isometries* (or unitaries, or channels) do not, because of the requirement for suitable composition presented in Section 3.1.3, which makes it illegal in some cases to sequentially compose two routed isometries. Our desire to stay within circuit theories is thus not entirely fulfilled. We see this as an unfortunate but unavoidable feature of any attempt at capturing the phenomenon of quantum control (we discuss why in Section 6.2.1). What we achieve here is to minimise the trouble that this brings about, by showing that sequential composition of physical maps is safe as long as simple conditions, involving the routes only, are checked. In Section 3.4, and later in Chapter 5, we will show how, alternatively, some *global* conditions on a circuit can be checked to ensure its consistency.

Fortunately, the basic ingredients for our framework can be found already in the recent literature; in fact, in Chapter 2 we took care to present the latter in a way that puts emphasis on these ingredients. The first one of these is the idea of *sectorial constraints and correlations* which we used to describe the superposition of trajectories (Section 2.2). The second is the diagrammatic notation introduced, in an informal way, in the study of causal decompositions (Section 2.3). As we shall see, all that is left for us to do is to give these ideas a proper mathematical description, and to turn this description into a general framework.

The way we will make these ideas formal is by encoding the sectorial constraints explicitly, using maps in the theory of relations (or equivalently, of Boolean matrices); this yields *routes*. Supplementing our theory with routes is sufficient to generate a framework that satisfies all of our demands: it forms a circuit theory, allows for intuitive diagrammatic notation, specifies the correct Hilbert spaces in use, and features simple theorems ensuring the preservation of physicality. In particular, we shall see that sectorial constraints can also be used to enforce sectorial correlations. Furthermore, the framework can be extended in a natural way to the case of noisy quantum evolutions, modelled using completely positive maps. Finally, the index-matching diagrams of Ref. [55] can be recovered as a specific sub-theory in which a more intuitive diagrammatic notation is available, and in which preservation of physicality can be checked in an easy way.

The structure of this chapter is as follows. In Section 3.1, we present the framework of routed maps in the case of pure quantum theory, prove that it allows for a consistent diagrammatic representation, and show it in action by means of an example. In Section 3.2, we describe the kinds of diagrams this framework leads to, and their interpretation. In Section 3.3, we extend our framework to encompass general quantum channels, and illustrate with an example how it leads to natural decoherence computations. Finally, in Section 3.4, we show how a sub-framework yields the index-matching quantum circuits of Ref. [55], endowing them with a sound and systematic semantics.

3.1 Routed maps for pure quantum theory

We will first present *routed linear maps* (or routed maps for short), which can be used to describe pure quantum theory (i.e. for pure states and isometric channels). Routed maps come from the introduction of routes, which are mathematical objects encoding sectorial constraints on linear maps.

3.1.1 Sectorial constraints and routes

We need a mathematical tool to efficiently and compactly encode sectorial constraints. As we will display here, the relevant notion is that of a *relation*.

But in order to talk about sectorial constraints, one first has to work with spaces that are formally partitioned into sectors. We want to define a *sectorised space* as

a (finite-dimensional) Hilbert space $\mathcal{H}_A$ partitioned into orthogonal subspaces, i.e. $\mathcal{H}_A = \bigoplus_{k \in \mathcal{Z}_A} \mathcal{H}_A^k$, with $\mathcal{Z}_A$ a finite set. A practical way to define sectorisations is to use the orthogonal projectors onto the sectors: we say that a family $\left(\pi_A^k\right)_{k \in \mathcal{Z}}$ of orthogonal projectors on a finite-dimensional Hilbert space $\mathcal{H}_A$ defines a sectorisation of $\mathcal{H}_A$ if $\forall k, l,\ \pi_A^k \circ \pi_A^l = \delta^{kl} \pi_A^k$ and $\sum_k \pi_A^k = \mathrm{id}_A$. The length of this sectorisation is the size of $\mathcal{Z}_A$.

A sectorised space can then be formally defined:

Definition 3.1.1 (Sectorised Hilbert space)**.** *A (finite-dimensional) sectorised Hilbert space is a tuple $\left(\mathcal{H}_A, \mathcal{Z}_A, \left(\pi_A^k\right)_{k \in \mathcal{Z}_A}\right)$ where $\mathcal{H}_A$ is a finite-dimensional Hilbert space, $\mathcal{Z}_A$ is a finite set of index values, and $\left(\pi_A^k\right)_{k \in \mathcal{Z}_A}$ is a sectorisation of $\mathcal{H}_A$.*

We will colloquially refer to such a sectorised space by the name A^k. Note how the k superscript, in this notation, does not refer to a specific value of the sector index; on the contrary, it is there to indicate that there are several values to pick. This is in analogy with the Einstein notation for tensors, where one writes $g_{\mu\nu}$ to denote an entire matrix, and not a specific coefficient in it.

It is important to stress that in the framework we are building, sectorisations are hardcoded: formally, two different sectorisations of the same space give rise to two different sectorised spaces, which should not be confused with each other. From two sectorised spaces $A^k = \left(\mathcal{H}_A, \mathcal{Z}_A, \left(\pi_A^k\right)_{k \in \mathcal{Z}_A}\right)$ and $B^l = \left(\mathcal{H}_B, \mathcal{Z}_B, \left(\mu_B^l\right)_{l \in \mathcal{Z}_B}\right)$, one can form their tensor product $A^k \otimes B^l := \left(\mathcal{H}_A \otimes \mathcal{H}_B, \mathcal{Z}_A \times \mathcal{Z}_B, \left(\pi_A^k \otimes \mu_B^l\right)_{(k,l) \in \mathcal{Z}_A \times \mathcal{Z}_B}\right)$.

Given two sectorised spaces A^k and B^l, sectorial constraints on linear maps $A^k \to B^l$ can be encoded by a set of arrows from the elements of $\mathcal{Z}_A$ to those of $\mathcal{Z}_B$, where the absence of an arrow between two elements means that the sectors they label are forbidden to be connected. For example, if the sectors of A^k are labelled by $\mathcal{Z}_A = \{1, 2, 3, 4\}$, and those of B^l by $\mathcal{Z}_B = \{a, b, c, d\}$, a possible set of constraints λ is represented by the graph

$$\tag{3.1}$$
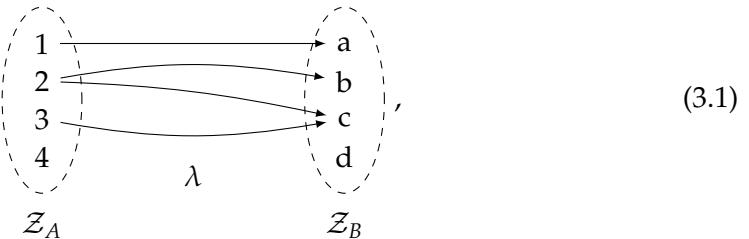
which encodes the following constraints on a linear map $f : \mathcal{H}_A \to \mathcal{H}_B$:

$$
\begin{cases}
f\left(\mathcal{H}_A^1\right) \subseteq \mathcal{H}_B^a\,; \\
f\left(\mathcal{H}_A^2\right) \subseteq \mathcal{H}_B^b \oplus \mathcal{H}_B^c\,; \\
f\left(\mathcal{H}_A^3\right) \subseteq \mathcal{H}_B^c\,; \\
f\left(\mathcal{H}_A^4\right) = \{0\}\,.
\end{cases}
\tag{3.2}
$$

Note how the sectorial constraints, among other things, entail that f must be null on sector $\mathcal{H}_A^4$.

Graphs of the form of (3.1) correspond to mathematical objects called *relations*. Relations are a way of modelling connections between elements of two sets; they can be thought of as generalisations of functions, in which a given element of the input set can be mapped to any number of elements of the output set (including the possibility that it is mapped to no element at all) [103]. For example, λ, as represented by (3.1), is a relation from $\mathcal{Z}_A$ to $\mathcal{Z}_B$.

The fact that λ relates $k \in \mathcal{Z}_A$ to $l \in \mathcal{Z}_B$ is denoted $k \overset{\lambda}{\sim} l$: here, for instance, $2 \overset{\lambda}{\sim} b$, $2 \overset{\lambda}{\sim} c$, etc. Relations can be sequentially composed in a natural way, following the rule that two elements are related if there exists at least one path between them:

$$
\begin{array}{c}
\text{(3.3)}
\end{array}
$$
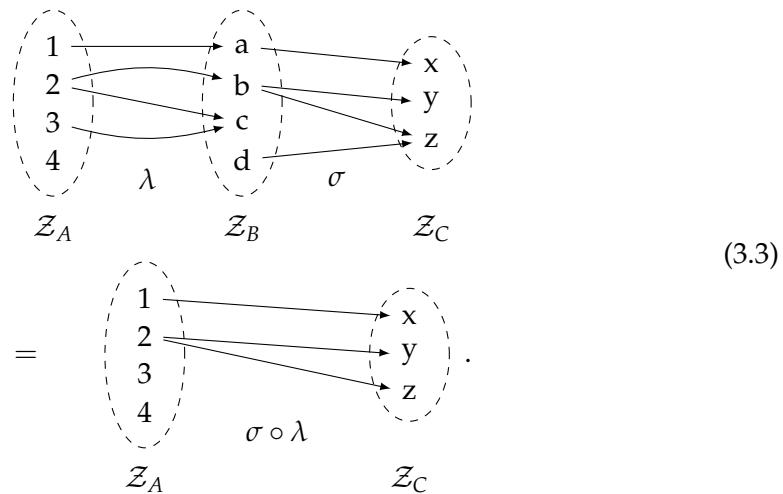
Relations can be parallelly composed using cartesian products, with the rule: $(k_1, k_2) \overset{\lambda_1 \times \lambda_2}{\sim} (l_1, l_2)$ if and only if $k_1 \overset{\lambda_1}{\sim} l_1$ and $k_2 \overset{\lambda_2}{\sim} l_2$. Finally, from a relation $\lambda : \mathcal{Z}_A \to \mathcal{Z}_B$, one can define the opposite relation $\lambda^\top : \mathcal{Z}_B \to \mathcal{Z}_A$, given by reversing the arrows in λ's graph.

A relation λ can equivalently be represented by a matrix[2] $\left(\lambda_k^l\right)_{k \in \mathcal{Z}_A, l \in \mathcal{Z}_B}$ with coefficients in the semiring of booleans: $\lambda_k^l = 1$ if $k \overset{\lambda}{\sim} l$, and 0 otherwise. In this picture, sequential composition is given by matrix products, parallel composition by tensor products of matrices, and taking the opposite relation corresponds to matrix transposition. In the rest of this paper, we will predominantly work with the representation of relations as boolean matrices, and refer to a relation λ by its boolean components λ_k^l; note how this is once again reminiscent of the Einstein notation for tensors.

A route is a relation that represents a set of sectorial constraints: the constraint that a sector $\mathcal{H}_A^k$ of the input space is forbidden from being connected to a sector $\mathcal{H}_B^l$ of the output space will be denoted by the fact that λ features no arrow from k to l, or equivalently, $\lambda_k^l = 0$. For example, if we take the sectorised Hilbert spaces $\mathcal{H}_A = \mathcal{H}_A^0 \oplus \mathcal{H}_A^1$ and $\mathcal{H}_B = \mathcal{H}_B^0 \oplus \mathcal{H}_B^1$, the constraint that a linear map $f : \mathcal{H}_A \to \mathcal{H}_B$

---

[2]To improve clarity, we will follow the convention of writing input indices in subscript and output indices in superscript.

satisfies $f(\mathcal{H}_A^1) \subseteq \mathcal{H}_B^1$ (i.e. f does not connect $\mathcal{H}_A^1$ to $\mathcal{H}_B^0$) will be represented by the route $\lambda = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$. Formally, we have:

Definition 3.1.2 (Routes). *Let* $\left(\mathcal{H}_A, \mathcal{Z}_A, (\pi_A^k)_{k \in \mathcal{Z}_A}\right)$ *and* $\left(\mathcal{H}_B, \mathcal{Z}_B, (\mu_B^l)_{l \in \mathcal{Z}_B}\right)$ *be two sectorised spaces, and* $\lambda : \mathcal{Z}_A \to \mathcal{Z}_B$ *a relation. A linear map* $f : \mathcal{H}_A \to \mathcal{H}_B$ ***follows the route*** λ *if*

$$f = \sum_{lk} \lambda_k^l \cdot \mu_B^l \circ f \circ \pi_A^k. \tag{3.4}$$

One also says that λ ***is a route*** *for* f.

An equivalent condition to (3.4), proven in Appendix A.3.2, is

$$\forall k, l, \; \lambda_k^l = 0 \implies \mu_B^l \circ f \circ \pi_A^k = 0. \tag{3.5}$$

This yields an intuitive interpretation of routes: the 1's in the matrix of a route λ can be thought of as designating the blocks that are allowed to be non-zero in the block decomposition of f.

An important fact is that, on sectorised Hilbert spaces, compatibility of linear maps with routes plays well with sequential composition, parallel composition, and hermitian adjoints: if f follows λ and g follows σ, then $g \circ f$ follows $\sigma \circ \lambda$, $f \otimes g$ follows $\lambda \times \sigma$, and $f^\dagger$ follows $\lambda^\top$. This is proven in Appendix A.3.2.

3.1.2 Routed linear maps

We are now in a position to define routed maps, which, together with sectorised spaces, form the basic components of our framework:

Definition 3.1.3 (Routed maps). *A **routed linear map** (or routed map for short) from A^k to B^l is a pair (λ, f) where $\lambda : \mathcal{Z}_A \to \mathcal{Z}_B$ is a relation, and $f : \mathcal{H}_A \to \mathcal{H}_B$ is a linear map which follows λ.*

For example, if we go back to the scenario described in Section 2.2 (restricting for now to the pure version, in which all operations are unitary operators), Alice and Bob's wires and operations can be modelled, respectively, as sectorised spaces of the form $\mathcal{H} = \mathcal{H}^0 \oplus \mathcal{H}^1$, and as routed maps of the form (δ, V), where $\delta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ encodes the constraint of sector preservation (corresponding here to preservation of the number of particles), and V is a unitary map (which, by definition, has to follow the route δ).

Routed maps themselves can be sequentially and parallelly composed, through pairwise composition in both cases,[3] and one can take their hermitian adjoint: $(\lambda, f)^\dagger :=$

---

[3]Note that, because sectorisations are hardcoded into sectorised spaces, one can sequentially compose two routed maps only if the first map's output space is equal to the second map's input space, *including the sectorisation*.

$(\lambda^\top, f^\dagger)$. These features are all encompassed formally by Theorem A.3.1, stated and proven in Appendix A.3.2, which, more generally, characterises the framework of sectorised Hilbert spaces and routed linear maps as a †-symmetric monoidal category. This has another important practical consequence: routed maps can be represented graphically in a well-defined way using circuit diagrams. Circuit diagrams where the wires are interpreted as sectorised Hilbert spaces and the boxes are interpreted as routed linear maps shall be referred to as routed quantum circuits, or simply, routed circuits.

Formally, we have:

Theorem 3.1.1. *The framework of sectorised Hilbert spaces and routed linear maps admits a sound representation in terms of circuit diagrams.*

Proof. This follows from Theorem A.3.1, of Appendix A.3.2, and the fact that symmetric monoidal categories are suitable for diagrammatic representation in terms of circuit diagrams [11, 60]. □

Soundness in Theorem 3.1.1 means the following. We take two circuit diagrams whose wires are interpreted as sectorised Hilbert spaces and whose boxes are interpreted as routed linear maps; if these are provably equal as diagrams (i.e. if one can be obtained by simply deforming the other), then the routed linear maps they represent are provably equal [11]. Essentially, this should be understood as ensuring that circuit diagrams can be used without second thoughts when dealing with routed linear maps, just as they could be used without second thoughts when dealing with standard linear maps.

Note that in Appendix A.1, we provide additional comments on how the 'route' part of a routed map can be understood at the conceptual level.

3.1.3   Routed isometries

An important task is to single out those routed maps which correspond to physical evolutions. In the standard framework of quantum circuits for pure quantum theory, they are given by isometries; for routed maps, we will instead coin the notion of *routed isometries*. It is important to understand how this notion comes about; two remarks explain it.

The first remark is that the isometricity condition, $h^\dagger \circ h = \mathrm{id}$, should not be imposed on the 'route' part of a routed map (λ, f); in other words, one should *not* ask that $\lambda^\top \circ \lambda = \mathrm{id}$. This is because this route part is there solely to encode constraints on the physical evolution, not the physical evolution itself; there is no reason for it to satisfy isometricity – which can be thought of as enforcing the non-disparition of information in the evolution.

The second remark is that one of the main uses of route is to encode the fact that some input or output sectors are, in fact, never used – as we shall soon see in applications, this is how they can be used to enforce sectorial correlations. An example is

the λ of (3.1), which connects the input value '4' to no output value, effectively forcing maps to be null on this sector. This should be understood as expressing the fact that, in the physical scenario at hand, this sector is never populated, and that it is only present for formal convenience. For a linear map U that follows λ, physicality should thus only be checked on the other sectors. We will characterise the latter as being the 'practical inputs' of λ.

For a routed map $(\lambda, U) : A^k \to B^l$, we define the *practical input set* of λ, $\mathcal{S}_\lambda$, as the subset of $\mathcal{Z}_A$ whose elements are related by λ to at least one element of $\mathcal{Z}_B$ (for example, for λ as defined in (3.1), we have $\mathcal{S}_\lambda = \{1, 2, 3\}$). We define the corresponding *practical input space* of (λ, U) as $\mathcal{H}_A^{\mathcal{S}_\lambda} := \bigoplus_{k \in \mathcal{S}_\lambda} \mathcal{H}_A^k$. The symmetric notions of practical output set $\mathcal{T}_\lambda$ and practical output space $\mathcal{H}_B^{\mathcal{T}_\lambda}$ are defined in the same way. This enables us to spell out the proper notion of an isometry – and of a unitary – for routed maps.

Definition 3.1.4. *Let (λ, U) be a routed map from A^k to B^l, with practical input space $\mathcal{H}_A^{\mathcal{S}_\lambda}$. (λ, U) is a **routed isometry** if U is an isometry when restricted to $\mathcal{H}_A^{\mathcal{S}_\lambda}$. (λ, U) is a **routed unitary** if both (λ, U) and $(\lambda, U)^\dagger$ are routed isometries.*

Equivalently, (λ, U) is a routed isometry if U is a partial isometry with initial domain $\mathcal{H}_A^{\mathcal{S}_\lambda}$. Similarly, (λ, U) is a routed unitary if U is a partial isometry with initial domain $\mathcal{H}_A^{\mathcal{S}_\lambda}$ and with range $\mathcal{H}_B^{\mathcal{T}_\lambda}$.

In the routed maps framework for pure quantum theory, the physically meaningful routed maps are the routed isometries. One, however, has to be careful on one point: the sequential composition of two routed isometries is not necessarily a routed isometry itself. The badly-behaved compositions of routed isometries correspond to situations in which we have complete descriptions for two individual gates, but where these descriptions are not sufficient to specify a complete description of the sequential composition of these two gates. Parallel compositions of routed isometries, on the other hand, always yield routed isometries, as proven in Appendix A.4.

We therefore need to single out the sequential compositions which are well-behaved for routed isometries. We can do so with a condition which, crucially, depends solely on the maps' routes:

Theorem 3.1.2. *Let $\lambda : \mathcal{Z}_A \to \mathcal{Z}_B$ and $\sigma : \mathcal{Z}_B \to \mathcal{Z}_C$ be two routes satisfying*

$$\left(\lambda \circ \lambda^\top \right) [\mathcal{S}_\sigma] \subseteq \mathcal{S}_\sigma. \tag{3.6}$$

Then, for any routed isometries $(\lambda, U) : A^k \to B^l$ and $(\sigma, V) : B^l \to C^m$, their composition $(\sigma, V) \circ (\lambda, U)$ is a routed isometry.

Proof. See Appendix A.4. □

When the condition (3.6) is satisfied, we say that the sequential composition of λ and σ is *proper for routed isometries*.

Theorem 3.1.2 and its forthcoming generalisation to quantum channels are the crucial consistency theorems for routed quantum circuits. In routed quantum circuits made of routed isometries, all sequential compositions have to satisfy (3.6), in order to ensure that the global map they form is also a routed isometry. For the case of routed unitaries, sequential composition is well-behaved if the routes satisfy both (3.6) and a symmetric condition:

Theorem 3.1.3. *Let $\lambda : \mathcal{Z}_A \to \mathcal{Z}_B$ and $\sigma : \mathcal{Z}_B \to \mathcal{Z}_C$ be two routes satisfying*

$$\left(\lambda \circ \lambda^\top\right)[\mathcal{S}_\sigma] \subseteq \mathcal{S}_\sigma\,, \tag{3.7a}$$

$$\left(\sigma^\top \circ \sigma\right)[\mathcal{T}_\lambda] \subseteq \mathcal{T}_\lambda\,. \tag{3.7b}$$

Then, for any routed unitaries $(\lambda, U) : A^k \to B^l$ and $(\sigma, V) : B^l \to C^m$, their composition $(\sigma, V) \circ (\lambda, U)$ is a routed unitary.

Under these conditions, we say that the sequential composition of λ and σ is *proper for unitaries*.

The previous conditions characterise the valid *constructions* of routed circuits: to prove that a circuit is valid, one has to build it step by step, through sequential and parallel compositions, checking that the former are always proper for the type of map considered (a discussion of why this is necessary is available in Section 6.2.1). Another possible verification method would be a 'global' one, in which one would directly analyse the circuit as a whole. As we shall see later on, this can be done in a very simple way for a subclass of routed circuits called *index-matching routed circuits*. Furthermore, in Chapter 5, we will also provide such a method for general circuits; it will be primarily aimed at certifying the consistency of routed circuits that feature feedback loops, but it can also, as a special case, be applied to standard routed circuits such as the ones studied in the present chapter.

3.1.4   An example: superposition of two trajectories

Before we move on to the case of general quantum channels, let us provide a first didactic example of a routed circuit, by showing how our framework allows us to properly formalise the scenario of a superposition of two trajectories described in Section 2.2 – restricting for now to the case of unitary channels. Diagrammatically, we represent sectorised spaces as wires, and routed maps as boxes: we write the linear map within the box, and depict the matrix elements of its route floating next to it. Spaces with a trivial sectorisation are denoted without superscripts. The scenario is then formalised as the following routed circuit:

$$
\begin{array}{c}
\text{(diagram)}
\end{array}
\tag{3.8}
$$
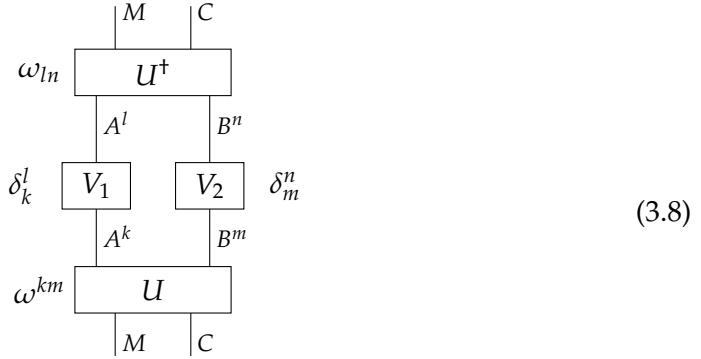
where $\omega = \begin{pmatrix} 0 & 1 & 1 & 0 \end{pmatrix}$, and $\delta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

As we can see, Alice and Bob's channels are now represented as routed maps of the form (δ, V), in which the sectorial constraints inherent to the scenario have been included. Let us also carefully break down the meaning of the encoding operation, (ω, U). As the input wires of this operation are not sectorised, ω is a relation from a trivial set of indices – represented by the singleton $\{*\}$ – to the set $\mathcal{Z}_A \times \mathcal{Z}_B = \{(0,0), (0,1), (1,0), (1,1)\}$. ω's graph is
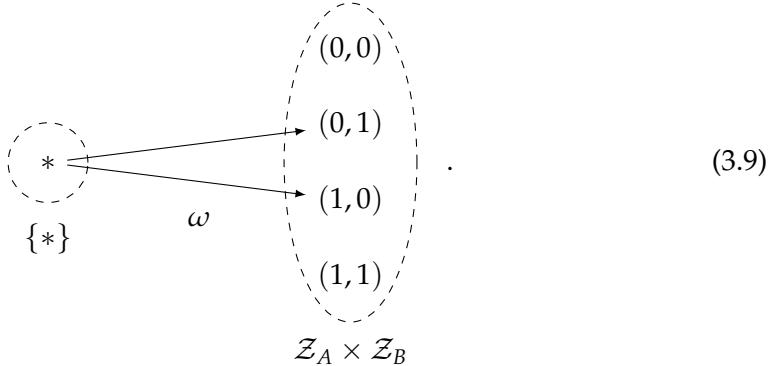
As we can see, ω is characterised by its practical output set $\mathcal{T}_\omega = \{(0,1), (1,0)\}$. (ω, U)'s practical output space, $\mathcal{H}_{AB}^{\mathcal{T}_\omega}$, is thus precisely the $\widetilde{\mathcal{H}}_{AB}$ introduced in section 2.2: this enforces the sectorial correlations present in the scenario. It is important to stress that within the framework of routed maps, these sectorial correlations are obtained as a contextual feature (see footnote 5 about our use of the word 'contextual'): they are specified by the routes present in the global routed circuit. This point is elaborated upon in Section 3.2.3.

All the routed maps in this routed circuit are routed unitaries, and it is easy to check that all the compositions are proper for routed unitaries. This means that the framework of routed maps allowed us to provide a suitable unitary description of this unitary scenario – something which, as we argued in section 2.2, is not possible within the sole framework of standard quantum circuits. More generally, it is straightforward to see that the use of routed maps solves all the points of dissatisfaction we had with the description of this scenario in standard quantum circuits.

One can reduce graphical clutter in the above routed circuit by using a handy

graphical convention, that of contracting Kronecker deltas. The idea is, not to write explicitly the δ-routes δ_k^l between a wire A^k and a wire A^l, and to instead just write down these wires with the same superscript.[4] This is in analogy with index repetition in the Einstein convention. (3.8), for example, then becomes:

$$
\begin{array}{c}
\quad\;\; \big|M \quad \big|C \\[2pt]
\omega_{km} \;\boxed{\quad U^\dagger \quad} \\[2pt]
\quad A^k \qquad B^m \\[2pt]
\boxed{V_1} \qquad \boxed{V_2} \\[2pt]
\quad A^k \qquad B^m \\[2pt]
\omega^{km} \;\boxed{\quad U \quad} \\[2pt]
\quad\;\; \big|M \quad \big|C
\end{array}
\tag{3.10}
$$
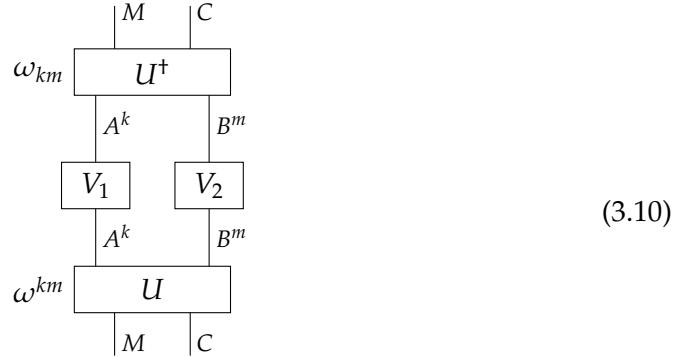
3.2 Diagrammatic representation: routed circuits

Let us provide a thorough description of the diagrammatic representation that we just introduced in a simple example. Indeed, one of the objectives of the introduction of routed maps is to use them as a mathematical basis for a faithful and systematic diagrammatic representation, in which the routes can be read in an intuitive way. We provide such a representation in the form of so-called *routed circuits*. The well-definition of these diagrams as a faithful representation of the mathematical framework is guaranteed by Theorem 3.1.1. A specific challenge in this context is to give clear rules on the physical interpretation of slices in a given routed circuit: we will do so by establishing a distinction between *formal space* and *accessible space*.

3.2.1 Diagrams for routed linear maps

An example of a routed circuit is (3.8). We represent the objects $X^k := (\mathcal{H}_X, \mathcal{Z}_X, (\pi_X^k)_{k \in \mathcal{Z}_X})$ by wires. We represent the morphisms (λ, f) by boxes: we write the linear maps f inside the boxes, whereas the matrix elements of the route, $\lambda_{k,\ldots,l}^{m,\ldots,n}$, are drawn as numbers floating next to the boxes. In general, we ask that no two wires bear the same superscript (except in the case of the shorthand notation given by contractions of Kronecker deltas). When $|\mathcal{Z}_X| = 1$, we simply write X in place of X^k.

Remember that a diagram composed of routed isometries represents a routed isometry itself if and only if the sequential compositions of routes in this diagram are suitable for isometries, as per Theorem 3.1.2. In this case, the diagram is called an iso-diagram. In the same way, a diagram in which sequential compositions of routes are suitable for unitaries is called a uni-diagram.

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[4]Contraction of Kronecker deltas can sometimes lead to ambiguities about the routes in a given diagram (this will be elaborated upon in Section 3.4); one should therefore keep in mind that it is simply a graphical shorthand, and that the rigorous diagrammatic representation of routed quantum circuits is properly done through explicitly writing down all the routes.

3.2.2 How to interpret slices

An important question is that of the interpretation of slices in a diagram: it corresponds to our crucial requirement that the framework should allow us to determine the Hilbert spaces in actual use. By slices, we mean horizontal combinations of wires. For example, if we take the slice comprising wires A^k and B^m in (3.8), a simple formulation of the question at hand would be: 'What is the Hilbert space corresponding to this slice?'. As we will show, the answer depends on whether one is asking from a mathematical or physical perspective. This will lead us to distinguishing two spaces corresponding to a slice: the formal space, and the accessible space.

A first possible answer comes from strictly sticking to the mathematical formalism. As is clear from its definition in Section 3.1.2, the tensor product $A^k \otimes B^m$ has Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B = \bigoplus_{k,m} \mathcal{H}_A^k \otimes \mathcal{H}_B^m$. We will define this as the *formal space* corresponding to the slice. In contrast to what will come later, the formal space corresponding to a slice is non-contextual,[5] in the sense that it only depends on the slice itself. As we can see, the formal space is the 'oversized' Hilbert space discussed in Section 2.2.2: it contains all the sectors of the sectorisation.

It is clear, however, that some of these sectors are in general forbidden from being populated, due to the sectorial constraints imposed by the routes. Thus, in the context of the diagram at hand, one can give a more refined meaning to the slice. This is formalised by the notion of the *accessible space* corresponding to a slice: we define it as the subspace of the formal space in which states will be constrained to lie due to the routes. The accessible space corresponds to a more physical understanding of the situation, and encodes physical correlations between sectors in each of the wires which compose it. For example, the accessible space corresponding to the slice comprising wires A^k and B^m in (3.8) is $\mathcal{H}_A^1 \otimes \mathcal{H}_B^0 \oplus \mathcal{H}_A^0 \otimes \mathcal{H}_B^1$, a strict subspace of its formal space. As we see, the notion of accessible space recovers the Hilbert space $\tilde{\mathcal{H}}_{AB}$, the 'actual' Hilbert space at hand as argued in Section 2.2.2. We give the general recipe for computing the accessible Hilbert space corresponding to a slice in section 3.2.3.

Before that, it is important to emphasise that the accessible space is a *contextual* notion: it depends on the whole diagram (more specifically, on the routes thereof) and not only on the slice itself. This somewhat counter-intuitive feature should not come as a surprise. To see why, it is enlightening to take the view in which routed circuits are understood as representing a physical setup and the sectorial constraints this setup implies (this is for example the case in (3.8)). In this context, the whole point of the notion of accessible space is to take into account the fact that some setups lead to only a subspace of a given formal space being populated. It is thus natural that the whole setup should be taken into account when computing the accessible

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[5]Here, we use the word 'contextual' in a colloquial sense; this should not be confused with its use in discussions of non-contextuality as a quantum feature, in which 'contextuality' has a different, more technical meaning.

space.[6]

That the notion of accessible space is a contextual one entails another important consequence: the accessible space of a given slice can get modified (and, more specifically, reduced) when additional maps are adjoined to a diagram. For example, if one considers a diagram containing only the middle layer of (3.8), then the accessible space of the slice comprising wires A^k and B^m is equal to its formal space; but when one adjoins the other layers to recover the diagram above, this accessible space gets reduced to $\mathcal{H}_A^1 \otimes \mathcal{H}_B^0 \oplus \mathcal{H}_A^0 \otimes \mathcal{H}_B^1$. Once again, this is in fact natural: in the physical interpretation of routed maps, adding more routed maps means specifying a setup further - which could mean that we are adding new constraints on the possible physical correlations in a given slice.[7]

3.2.3 Computing the accessible space corresponding to a slice

An example of a more elaborate routed circuit, with slices explicitly drawn out, is given below; we will use this as an example to illustrate the general procedure which yields the accessible space corresponding to a slice. Two possible slices are drawn in blue and magenta, and their respective accessible Hilbert spaces are written out on the side:

$$\bigoplus_{ij} \eta^{ij} \mathcal{H}_E^i \otimes \mathcal{H}_F^j$$
$$\eta^{ij} := \sum_{mnkp} \delta_m^i \gamma_n^j \lambda_k^{mn} \alpha_p^k$$

$$\bigoplus_{in} \eta'^{in} \mathcal{H}_E^i \otimes \mathcal{H}_D^n \otimes \mathcal{H}_B$$
$$\eta'^{in} := \sum_{mkjp} \delta_m^i \lambda_k^{mn} \gamma_n^j \alpha_p^k$$

(3.11)

One can compute the accessible space corresponding to a given slice with the following formal procedure (using the blue slice above as an example). We call $\mathcal{K}$ the set of indices present in this slice [e.g. $\mathcal{K} = \{i, j\}$]. This procedure is justified more formally in Appendix A.5.

1. write down the matrix components of all the routes featuring an index in $\mathcal{K}$ [e.g. $\delta_m^i \gamma_n^j$];

---

[6]The considerations of Section 6.2.1 also shed some light on this issue, in particular on why it is an unavoidable one.

[7]There is a specific case of interest, however, in which the previous comment will not apply: when one is considering a diagram whose global input and output wires (the inputs and outputs of the whole diagram) are not sectorised (i.e. bear no indices). It is easy to see that adjoining more routed maps to such a diagram will not modify the accessible space of a given slice inside it; one can thus consider the accessible space to be the exact subspace which will be populated. For example, this is the case for the slice comprising wires A^k and B^m in (3.8), as the global inputs and outputs in (3.8) bear no indices.

2. write down the matrix components of all the routes (both above and below the slice under consideration)[8] featuring an index among those already present [e.g. λ_k^{mn}];

3. iterate until there are no matrix components left to add under the previous rule;

4. sum over all indices present, except the ones in $\mathcal{K}$; this yields the components of a boolean matrix η with indices in $\mathcal{K}$ [e.g. $\eta^{ij} := \sum_{mnkp} \delta_m^i \gamma_n^j \lambda_k^{mn} \alpha_p^k$];

5. write down the explicit direct sum of all the sectors in the slice with η [e.g. $\bigoplus_{i,j} \eta^{ij} \mathcal{H}_E^i \otimes \mathcal{H}_F^j$]: this yields the accessible Hilbert space corresponding to the slice.

As one can see, this displays formal similarities with the Einstein summation convention of linear algebra. One should not take these similarities too seriously, however, as some conventions are different. In particular, in the formula for the accessible space, the indices in $\mathcal{K}$ appear three times, and indices born by input or output wires of the diagram appear one time yet are still summed over.

3.2.4   A (further) diagrammatic shorthand: global index constraints

Finally, we introduce a further diagrammatic shorthand, generalising index-matching in order to give a more compact and readable diagrammatic presentation of routed circuits. The idea is, rather than directly stating the route associated with each map in the circuit, to specify a *global index constraint*, from which the individual routes can be derived. This global index constraint specifies the allowed joint value-assignments for all of the indices in the circuit, allowing us in practice to get rid of the redundancy and obscurity that come about quickly when one has to define the routes individually.

Routed circuits with global index constraints feature (possibly repeated) indices on their wires, together with equations floating on the side, relating some of these indices. For instance, the relevant circuit for the superposition of trajectories is

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[8]It might sound surprising that the routes *above* (i.e. after) the slice should be taken into account as well, but this is in fact necessary: the consistency of the process formed by the whole diagram forces one to restrict the states which can populate a given slice so that they do not lie out of the practical input space of a subsequent routed map.

$$
\begin{array}{c}
\vert M \quad \vert C \\
\boxed{U^\dagger} \\
A^k \quad\quad B^m \\
\boxed{V_1} \quad \boxed{V_2} \qquad k + m = 1 \ . \\
A^k \quad\quad B^m \\
\boxed{U} \\
\vert M \quad \vert C
\end{array}
\tag{3.12}
$$
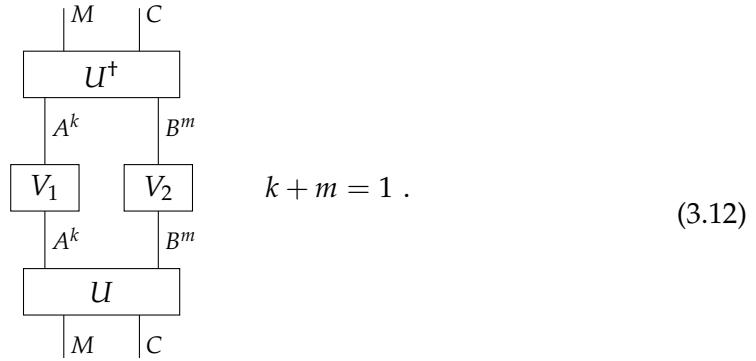
Taking $\mathcal{Z}^{\mathrm{tot}} := \bigtimes_A \mathcal{Z}_A$ to be the cartesian product of the sets of index values of every sectorisation present in the circuit, the equations together with the index-matching define a subset $\mathcal{Z}^{\mathrm{poss}} \subseteq \mathcal{Z}^{\mathrm{tot}}$ of joint values that satisfy them ('possible' joint values) – in (3.12), for instance, $\mathcal{Z}^{\mathrm{poss}} = \{(0,1,0,1),(1,0,1,0)\}$. One can then infer the route assigned to a given map by taking it to be the least restrictive route consistent with the global index constraint and the index-matching.

This can be defined formally in the following way. The global index constraint together with the index-matching yield a Boolean tensor $G_{\vec{k}}$ over the Cartesian product of all the indices in the graph: $G_{\vec{k}} = 1$ if the value assignment $\vec{k}$ satisfies them, and $G_{\vec{k}} = 0$ otherwise. Taking then a map f in the circuit, its associated route is defined as the marginalisation of G over all indices that do not appear in the inputs or outputs wires of f:

$$
\lambda^{\vec{k}_{\mathrm{out}}}_{\vec{k}_{\mathrm{in}}} := \sum_{\vec{k'}} G_{\vec{k}_{\mathrm{in}} \vec{k}_{\mathrm{out}} \vec{k'}} \, ,
\tag{3.13}
$$

where we have partitioned $\vec{k}$ into $\vec{k}_{\mathrm{in}}$ and $\vec{k}_{\mathrm{out}}$, the values of the indices appearing respectively in the input and outputs of f, and $\vec{k'}$, the values of the other indices in the circuit.

We want to stress, once again, that the use of index-matching and global index constraints is only a graphical shorthand: in order to make sense of the routed circuit, they have to be formally translated into routes for the nodes.

3.3 Routed maps for mixed quantum theory

3.3.1 Routed quantum channels

Let us now show how to extend the theory of routed maps to encompass mixed states and general quantum channels. In the same way that one goes from linear maps to completely positive linear maps, we will be going from relations to completely positive relations. These will be used to encode sectorial constraints which can not only forbid connections between some sectors, but also forbid some of the allowed connections to be coherent with one another.

The broad idea is to generalise (3.4) to the case where we take a completely positive linear map $\mathcal{C} : \mathcal{L}\left(\bigoplus_{k \in \mathcal{Z}_A} \mathcal{H}_A^k\right) \to \mathcal{L}\left(\bigoplus_{l \in \mathcal{Z}_B} \mathcal{H}_B^l\right)$ between linear operators on sectorised Hilbert spaces. A natural way to do so is to use relations of the form $\Lambda : \mathcal{Z}_A \times \mathcal{Z}_A \to \mathcal{Z}_B \times \mathcal{Z}_B$ as routes, leading to the following definition:

Definition 3.3.1 (Routes for CPMs). *Let $\left(\mathcal{H}_A, \mathcal{Z}_A, \left(\pi_A^k\right)_{k \in \mathcal{Z}_A}\right)$ and $\left(\mathcal{H}_B, \mathcal{Z}_B, \left(\mu_B^l\right)_{l \in \mathcal{Z}_B}\right)$ be two sectorised spaces, and $\Lambda : \mathcal{Z}_A \times \mathcal{Z}_A \to \mathcal{Z}_B \times \mathcal{Z}_B$ a relation. A completely positive map $\mathcal{C} : \mathcal{L}\left(\mathcal{H}_A\right) \to \mathcal{L}\left(\mathcal{H}_B\right)$ **follows** Λ if*

$$\forall \rho, \quad \mathcal{C}(\rho) = \sum_{ll'kk'} \Lambda_{kk'}^{ll'} \cdot \mu_B^l \circ \mathcal{C}\left(\pi_A^k \circ \rho \circ \pi_A^{k'}\right) \circ \mu_B^{l'}. \tag{3.14}$$

*One also says that Λ **is a route** for $\mathcal{C}$.*

However, we need not use all of the possible Λ's; some are superfluous. Take, for instance, a Λ which is not symmetric, in the sense that, for some k, k', l, l', $1 = \Lambda_{kk'}^{ll'} \neq \Lambda_{k'k}^{l'l} = 0$. As completely positive maps are symmetric, any $\mathcal{C}$ following Λ will also follow $\tilde{\Lambda}$ defined from Λ by setting $\tilde{\Lambda}_{kk'}^{ll'}$ to 0. In other words, a non-symmetric Λ expresses a set of constraints which could be expressed just as suitably by a symmetric one.

In addition, let us define the diagonal of Λ as the relation $\dot{\Lambda} : \mathcal{Z}_A \to \mathcal{Z}_B$ defined by $\dot{\Lambda}_k^l := \Lambda_{kk}^{ll}$. It is easy to see that if there exist k, l such that $\dot{\Lambda}_k^l = 0$, then any completely positive $\mathcal{C}$ that follows Λ will also follow the route $\tilde{\Lambda}$ obtained from the former by setting $\forall k', l', \tilde{\Lambda}_{kk'}^{ll'} = \tilde{\Lambda}_{k'k}^{l'l} = 0$. Let us define diagonally dominant relations Λ as the ones satisfying for any k, l, $\dot{\Lambda}_k^l = 0 \implies \forall k', l', \Lambda_{kk'}^{ll'} = \Lambda_{k'k}^{l'l} = 0$. This entails that a non diagonally dominant Λ expresses a set of constraints which could be expressed just as suitably by a diagonally dominant one. One can thus, without loss of generality, work only with symmetric and diagonally dominant Λ's.

Remarkably, the symmetric and diagonally dominant Λ's can be recovered in another way: they are exactly the *completely positive relations* that one can obtain by mimicking, on relations, the procedure that leads from linear maps to completely positive linear maps, through 'doubling then tracing out'. Indeed, one of the several equivalent definitions of completely positive linear maps is the following: $\mathcal{C} : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$ is a completely positive linear map if and only if it is of the form $\mathcal{C} : \rho \mapsto \mathrm{Tr}_E(M\rho M^\dagger)$, where $\mathcal{H}_E$ is an auxiliary Hilbert space and $M : \mathcal{H}_A \to \mathcal{H}_B \otimes \mathcal{H}_E$ is a linear map [11]. If, in an analogous way, we say that $\Lambda : \mathcal{Z}_A \times \mathcal{Z}_A \to \mathcal{Z}_B \times \mathcal{Z}_B$ is completely positive if there exists a set $\mathcal{Z}_E$ and a relation $\lambda : \mathcal{Z}_A \to \mathcal{Z}_B \times \mathcal{Z}_E$ such that $\Lambda_{kk'}^{ll'} = \sum_m \lambda_k^{lm} \lambda_{k'}^{l'm}$, then it can be found that a given Λ is a completely positive relation if and only if it is symmetric and diagonally dominant.[9] Sequential and parallel compositions of completely positive relations are completely positive relations.[10]

Completely positive relations will thus be used to express sectorial constraints for quantum channels, providing completely positive routes. The diagonal $\dot{\Lambda}_k^l$ of a

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[9]For a proof, see Ref. [104], Proposition 3.1.

[10]This follows directly from the universal CPM construction of Selinger [105].

completely positive route encodes constraints on whether a channel is allowed to connect the sectors k and l; and the off-diagonal coefficients $\Lambda_{kk'}^{ll'}$ encode constraints on whether the connections between sectors k and l on the one hand, and sectors k' and l' on the other hand, are allowed to be coherent with each other (these will be called *coherence constraints*).

In analogy with the construction for the pure case, routed CPMs are defined as follows, with sectorised spaces colloquially written as $\mathcal{L}\left(\bigoplus_{k\in\mathcal{Z}_A}\mathcal{H}_A^k\right) = \bigoplus_{k,k'\in\mathcal{Z}_A}\mathcal{L}(\mathcal{H}_A^k \to \mathcal{H}_A^{k'}) =: A^{kk'}$.

Definition 3.3.2 (Routed CPMs). *A **routed completely positive map (CPM)** from $A^{kk'}$ to $B^{ll'}$ is a pair $(\Lambda,\mathcal{C})$ where $\Lambda : \mathcal{Z}_A \times \mathcal{Z}_A \to \mathcal{Z}_B \times \mathcal{Z}_B$ is a completely positive relation, and $\mathcal{C} : \mathcal{L}\left(\bigoplus_{k\in\mathcal{Z}_A}\mathcal{H}_A^k\right) \to \mathcal{L}\left(\bigoplus_{l\in\mathcal{Z}_B}\mathcal{H}_B^l\right)$ is a completely positive map which follows Λ.*

The framework of sectorised Hilbert spaces and routed CPMs satisfies the exact analogue of Theorem 3.1.1:

Theorem 3.3.1. *The framework of sectorised Hilbert spaces and routed CPMs admits a sound representation in terms of circuit diagrams.*

Proof. This follows from Theorem A.3.3, of Appendix A.3.3, and from the fact that symmetric monoidal categories are suitable for diagrammatic representation in terms of circuit diagrams [11, 60]. □

Just as Theorem 3.1.1, this should be understood as ensuring that circuit diagrams can be used without second thoughts when dealing with routed CPMs.

Routed channels are defined in the same way as routed isometries, by asking them to be trace-preserving with respect to their practical input space.

Definition 3.3.3 (Routed quantum channels). *A routed CPM $(\Lambda,\mathcal{C}) : A^{kk'} \to B^{ll'}$ is a **routed quantum channel** if it is trace-preserving when restricted to act on its practical input space $\mathcal{L}(\mathcal{H}_A^{\mathcal{S}_{\dot{\Lambda}}})$, defined by the practical input set of Λ's diagonal, $\mathcal{S}_{\dot{\Lambda}}$.*

Finally, the condition for a composition of routed quantum channels to be proper (i.e., to always yield a routed quantum channel) is similar to that for routed isometries, and solely depends on their routes' diagonals:

Theorem 3.3.2. *Let $\Lambda : \mathcal{Z}_A \times \mathcal{Z}_A \to \mathcal{Z}_B \times \mathcal{Z}_B$ and $\Sigma : \mathcal{Z}_B \times \mathcal{Z}_B \to \mathcal{Z}_C \times \mathcal{Z}_C$ be two routes satisfying*

$$\left(\dot{\Lambda} \circ \dot{\Lambda}^\top\right)[\mathcal{S}_{\dot{\Lambda}}] \subseteq \mathcal{S}_{\dot{\Sigma}}. \tag{3.15}$$

Then, for any routed quantum channels $(\Lambda,\mathcal{C}) : A^{kk'} \to B^{ll'}$ and $(\Sigma,\mathcal{E}) : B^{ll'} \to C^{mm'}$, their composition $(\Sigma,\mathcal{E}) \circ (\Lambda,\mathcal{C})$ is a routed quantum channel.

The proof of this is similar to the one for routed isometries. When the condition (3.15) is satisfied, we say that the sequential composition of Λ and Σ is *proper for routed channels*.

3.3.2 Link with Kraus representations

A question of interest is whether the condition (3.14), expressing that a CP map $\mathcal{C}$ follows a completely positive route Λ, can be translated in terms of the Kraus representations $(K_i)_i$ of $\mathcal{C}$. A first answer is that the sectorial constraints expressed by Λ's diagonal $\dot{\Lambda}$ have to be satisfied by each of the Kraus operators in any Kraus decomposition of $\mathcal{C}$. This is also a sufficient condition when Λ has *full coherence*, i.e. when it is a route of the form $\Lambda^{ll'}_{kk'} = \dot{\Lambda}^l_k \dot{\Lambda}^{l'}_{k'}$ which includes no constraints on coherence:

Theorem 3.3.3. *Let* $\Lambda : \mathcal{Z}_A \times \mathcal{Z}_A \to \mathcal{Z}_B \times \mathcal{Z}_B$ *be a completely positive route, and* $\mathcal{C} : \mathcal{L}\left(\bigoplus_{k \in \mathcal{Z}_A} \mathcal{H}^k_A\right) \to \mathcal{L}\left(\bigoplus_{l \in \mathcal{Z}_B} \mathcal{H}^l_B\right)$ *a completely positive linear map, with a Kraus representation given by the set of operators* $(K_i)_i$*, where* $\forall i, K_i : \mathcal{H}_A \to \mathcal{H}_B$*.*

If $\mathcal{C}$ *follows* Λ*, then each of the* K_i*'s follow its diagonal* $\dot{\Lambda}$*. For a* Λ *with full coherence, the reverse implication holds as well.*

The other situation in which one can give conditions equivalent to (3.14) in terms of Kraus representations is the opposite extremal case: the one in which Λ is a route with *full decoherence*, i.e. is of the form $\Lambda^{ll'}_{kk'} = \delta_{kk'}\delta^{ll'}\dot{\Lambda}^l_k$. We say that a given Kraus decomposition $(K_i)_i$ is adapted to a completely positive route Λ with full decoherence if for each i, there exists a unique pair (k, l) such that $K_i = \mu^l_B \circ K_i \circ \pi^k_A$, i.e. K_i only maps from $\mathcal{H}^k_A$ to $\mathcal{H}^l_B$.

Theorem 3.3.4. *Let* $\Lambda : \mathcal{Z}_A \times \mathcal{Z}_A \to \mathcal{Z}_B \times \mathcal{Z}_B$ *be a completely positive route with full decoherence, and* $\mathcal{C} : \mathcal{L}\left(\bigoplus_{k \in \mathcal{Z}_A} \mathcal{H}^k_A\right) \to \mathcal{L}\left(\bigoplus_{l \in \mathcal{Z}_B} \mathcal{H}^l_B\right)$ *a completely positive linear map. Then* $\mathcal{C}$ *follows* Λ *if and only if there exists a Kraus representation of* $\mathcal{C}$ *adapted to* Λ*.*

Theorems 3.3.3 and 3.3.4 are proven in Appendix A.6.

3.3.3 Diagrammatic representation

Let us quickly elaborate on how the diagrammatic constructions and notions of Section 3.2 generalise to the case of mixed quantum theory. As exemplified in the next subsection, routed diagrams for mixed states and general quantum channels are in simple analogy with those for pure states and isometries: one simply switches to writing wires with doubled superscripts, of the form $A^{kk'}$, and to writing the completely positive routes with these same doubled indices. All compositions in such diagrams have to be suitable for routed quantum channels. The well-definition of these diagrams as a faithful representation of the mathematical framework is guaranteed by Theorem 3.3.1.

3.3.4 Two examples: Superposition of three trajectories and decoherence of copied information

We will exemplify the routed maps framework for general quantum channels with two examples to show how completely positive routes can include constraints on the coherence between sectors, and how this leads to easy decoherence computations.

In order to also present a somewhat more involved use of the routed circuits framework, let us extend the scenario we already formalised in Section 3.1.4, and consider now the superposition of three trajectories. This scenario is the same as before, except that the control system is now a qutrit, and the message can now go in a superposition of three different channels $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$, which once again preserve the number of particles [56].

Now that we are working with general quantum channels, there are in fact two different routes that one could attribute to $\mathcal{A}$ (and, in the same way, to $\mathcal{B}$ and $\mathcal{C}$); the choice between them depends on the features of the physical scenario we want to describe. On the one hand, we could be asking only that $\mathcal{A}$ preserves the number of particles, without setting constraints on the coherence between the vacuum sector and the one-particle sector. In this case, the route constraining $\mathcal{A}$ will be $\delta_k^l \delta_{k'}^{l'}$. But one could also be considering a more restrictive situation, in which $\mathcal{A}$ not only acts separately on the two sectors, but also acts incoherently on each [49, 56]. The choice of route corresponding to this situation is then $\delta_{kk'}^{ll'}$.[11] We see that the use of completely positive routes allows us to neatly distinguish between the two different scenarios.

Let us, for example, look at the scenario in which each channel is allowed to preserve coherence between the sectors. The routed circuit representing such a scenario (using contractions of Kronecker deltas) is then:

$$
\begin{array}{c}
\text{(3.16)}
\end{array}
$$
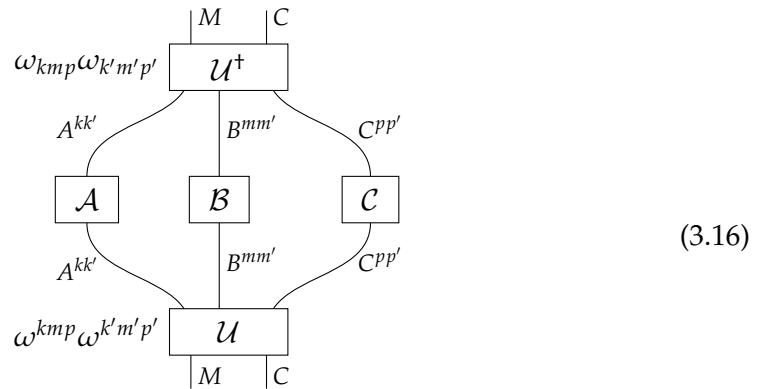
where, for given k, m and p, $\omega^{kmp} = 1$ if and only if $k + m + p = 1$. Remember that, because of the convention of contracting Kronecker deltas, writing the names of $\mathcal{A}$'s input and output wires with the same superscripts implicitly means that we are considering the routed quantum channel $(\delta_k^l \delta_{k'}^{l'}, \mathcal{A})$; the same goes with the routed quantum channels corresponding to Bob's and Charlie's actions.

On the other hand, in the scenario where the one-particle and vacuum sectors evolve incoherently with each other, the systems corresponding to Alice, Bob and Charlie would have repeated indices A^{kk}, B^{mm} and C^{pp}.

Another example shows how routes can help derive some immediate consequences of discardings on the coherence between sectors. Suppose we have a routed

---

[11]The Kronecker delta here means that $\delta_{kk'}^{ll'} = 1$ if and only if $l = l' = k = k'$, else $\delta_{kk'}^{ll'} = 0$.

channel from one system A to two sectorised systems $B^{kk'}$ and $C^{ll'}$, which features perfect (possibly coherent) sectorial correlations between $B^{kk'}$ and $C^{ll'}$ – i.e. this routed channel is of the form $(\delta^{kl}\delta^{k'l'}, \mathcal{C})$. This can be understood as a channel which, in particular, sends copies of the same information to two agents, Bob and Charlie. Indeed, if Bob measures in which of the sectors B^k his system is, and Charlie does the same with the sectors C^l, they will find the same result.

Let us now look at what happens if Bob discards his system (or, more generally, if Bob's system never reaches Charlie, as the latter's description of his own system is then the one obtained by discarding Bob's part). The discarding on $B^{kk'}$ is given by the routed quantum channel $(\delta_{kk'}, \stackrel{=}{\top}_B)$, where $\stackrel{=}{\top}_B$ is the trace on $\mathcal{L}(\mathcal{H}_B)$. The quantum channel this yields is therefore

$$
\begin{array}{ccc}
\delta_{kk'} \stackrel{=}{\top} & & \\
B^{kk'} \bigg| & \bigg| C^{ll'} & \bigg| C^{ll'} \\
\delta^{kl}\delta^{k'l'} \boxed{\;\mathcal{C}\;} & = & \delta^{ll'} \boxed{\;\mathcal{C}'\;} . \\
\big| A & & \big| A
\end{array}
\tag{3.17}
$$

In the equation above, some simple calculus on routes alone yielded an important physical theorem. Indeed, the routed quantum channel obtained by discarding Bob's system is of the form $(\delta^{ll'}, \mathcal{C}')$: its route means that it yields states that are completely decohered with respect to the sectorisation l. Thus we proved in a natural way a well-known feature of quantum theory: copying information and then discarding one of the copies necessarily leads to the loss of any coherence between the sectors which encoded this information in the other copy.

What is remarkable is that the use of completely positive routes allows us to derive such a theorem from very simple calculus on boolean matrices, and without having to know anything specific about the channel $\mathcal{C}$, except its crucial structural features. Moreover, the systematic nature of our framework means that one will be able to scale up such proofs easily: in any scenario in which information is copied in some way between any number of subsystems, for any number of subsystems being discarded, calculus on routes yields direct results on the coherence between sectors for the other subsystems.

3.3.5 Computing the accessible space corresponding to a slice

The discussion of interpretations of slices in a routed diagram can also be generalised to routed quantum channels. The formal space corresponding to a slice will, once again, be the 'big' space of linear operators corresponding to it: for example, the one corresponding to the slice comprising wires $A^{kk'}$, $B^{mm'}$ and $C^{pp'}$ in (3.16) is $\mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C)$. Accessible spaces will be defined as solely depending on the routes' diagonals: indeed, including the information on coherence encoded by the routes' off-diagonal elements would not yield satisfactory operator spaces. The

accessible space corresponding to the previously mentioned slice, for example, is
$\mathcal{L}[(\mathcal{H}_A^1 \otimes \mathcal{H}_B^0 \otimes \mathcal{H}_C^0) \oplus (\mathcal{H}_A^0 \otimes \mathcal{H}_B^1 \otimes \mathcal{H}_C^0) \oplus (\mathcal{H}_A^0 \otimes \mathcal{H}_B^0 \otimes \mathcal{H}_C^1)]$. Since we are only us-
ing the routes' diagonals, the accessible space corresponding to the same slice in the
incoherent case will be the same. The general procedure of Section 3.2.3 for comput-
ing the accessible space can easily be accommodated to general quantum channels:
one follows it using the routes' diagonals, thus ending up with a Hilbert space $\mathcal{H}^{\text{acc}}$;
the accessible space of linear operators corresponding to the slice is then $\mathcal{L}(\mathcal{H}^{\text{acc}})$.

3.3.6   A lighter notation in the absence of coherence constraints

When depicting scenarios in which only sectorial constraints are present, without
any coherence constraints, using completely positive relations becomes overkill. In-
deed, all the relations involved will then have full coherence and will be of the form

$$\Lambda_{kk'}^{ll'} = \dot{\Lambda}_k^l \dot{\Lambda}_{k'}^{l'}. \tag{3.18}$$

Such a Λ is characterised by its diagonal $\dot{\Lambda}$; the repetition of the latter in (3.18) is
a redundancy. For such scenarios, we can adopt a lighter notation in which this
redundancy is eliminated.

   The idea is to simply encode the sectorial constraints as single routes λ_k^l, and
to similarly write down the spaces as A^k, as in the framework for pure quantum
theory. One then says that a CP map $\mathcal{C}$ follows λ_k^l if, in the notation of Definition
3.3.1, it follows $\lambda_k^l \lambda_{k'}^{l'}$. As a reminder, this is the case if

$$\forall \rho, \quad \mathcal{C}(\rho) = \sum_{ll'kk'} \lambda_k^l \lambda_{k'}^{l'} \cdot \mu_B^l \circ \mathcal{C} \left(\pi_A^k \circ \rho \circ \pi_A^{k'} \right) \circ \mu_B^{l'}; \tag{3.19}$$

or equivalently, by Theorem 3.3.3, if all the operators in a Kraus decomposition of $\mathcal{C}$
follow λ (the choice of this Kraus decomposition being irrelevant).

   For example, with such a notation, the coherent superposition of three trajecto-
ries of (3.16) becomes

$$\tag{3.20}$$
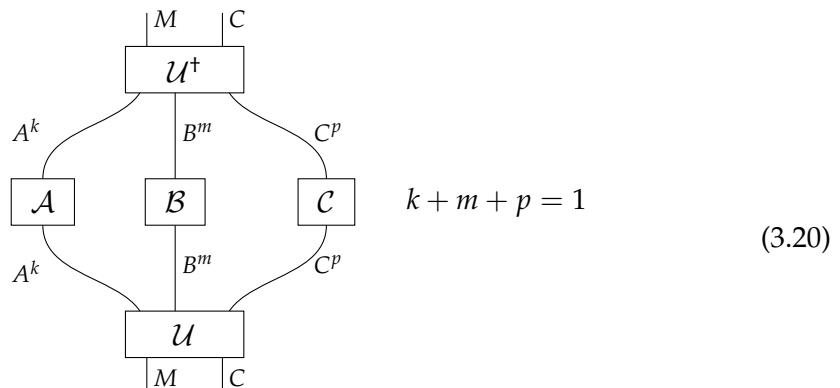
where we have also used the graphical shorthand of global index constraints intro-
duced in Section 3.2.4.

3.4 Index-matching quantum circuits

3.4.1 Motivation

A drawback of general routed quantum circuits is that the sectorial correlations and constraints they feature are not represented in a completely graphical way; the routes are denoted by abstract symbols which do not depict graphically the possible connections between sectors. Another issue is that the validity of a circuit for isometries or for unitaries has to be checked in an iterative way, by showing that the circuit can be built up from its elementary constituents while only using proper compositions.

Nevertheless, there is a sub-framework of routed quantum circuits which encompasses a fair share of scenarios (though not all of them), and in which these issues can be solved: this is the framework of *index-matching quantum circuits*. As we will see, index-matching quantum circuits correspond to the 'extended quantum circuits' introduced for the study of causal decompositions in Refs. [55, 69, 74, 75], and presented in Section 2.3. The theory of index-matching quantum circuits will thus also serve to provide a sound and systematic mathematical foundation to the use of the diagrams introduced in these earlier works.

The simple idea behind index-matching circuits is to make the most out of the graphical trick of Kronecker delta contraction, which we described earlier in a simple example. Thus, in this framework, one restricts the sectorisations to be indexed by a rigid combination of several indices, and only considers routes built from Kronecker deltas between such indices. This allows one to represent these routes directly on a diagram, by repeating indices to denote the Kronecker deltas. The conditions for suitable composition also take a particularly simple form in this context, making it easier to ensure that an index-matching circuit is suitable for routed isometries, routed unitaries, or routed channels. A typical example of an index-matching circuit is the causal decomposition (2.16).

3.4.2 A summary of the framework

We formalise thoroughly the framework of index-matching routed maps in Appendix A.7; here, we will present it in a more accessible way. At the level of pure states and operators, it has two major components. The first one is sectorised Hilbert spaces whose sectors are labelled by several indices, i.e. which are of the form $A^{k_1 \dots k_m}$. Each index k_i has a length $|k_i|$, denoting the number of values it can take. The second components is index-matching routed maps, which are routed maps whose route is solely written in terms of Kronecker deltas (in order to make sense, these Kronecker deltas necessarily have to relate indices of the same length). Examples of possible index-matching routes from $A^{k_1 k_2}$ to $B^{l_1 l_2}$ are $\delta_{k_1}^{l_1} \delta_{k_2}^{l_2}$, $\delta_{k_1 k_2}^{l_1 l_2}$, $\delta^{l_1 l_2}$, $\delta_{k_1 k_2}^{l_2}$, 1, etc.

Using graphical Kronecker delta contractions, the routes of index-matching routed maps can therefore be represented in a fully graphical way. For example, if we look
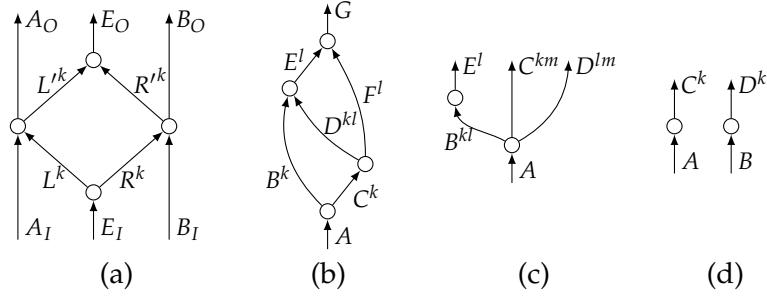
FIGURE 3.1: Examples of IODAGS.

at maps of type $A^{k_1} \otimes B^{k_2} \to C^{l_1} \otimes D^{l_2}$, the maps $(\delta^{l_1 l_2}_{k_1 k_2}, U_1)$, $(\delta^{l_1 l_2}, U_2)$ and $(1, U_3)$ will respectively be represented as

$$
\begin{array}{ccc}
\boxed{U_1} & \boxed{U_2} & \boxed{U_3}
\end{array}
\tag{3.21}
$$

Contractions of Kronecker deltas, however, can sometimes lead to ambiguities about the routes which are associated to each map in an index-matching circuit. For example, if we composed the channels $(\delta^{l_1}_{k_1} \delta^{l_2}_{k_2}, U) : A^{k_1} \otimes B^{k_2} \to C^{l_1} \otimes D^{l_2}$ and $(\delta^{m_1 m_2}_{l_1 l_2}, V) : C^{l_1} \otimes D^{l_2} \to E^{m_1} \otimes F^{m_2}$, this would lead to the index-matching circuit

$$
\begin{array}{c}
\boxed{V} \\
\boxed{U}
\end{array}
\tag{3.22}
$$

in which one now cannot properly read the first channel's route anymore, as it has been 'overwritten' by the route of the second channel. Such issues entail that, if we want to make sure we will be able to give an unambiguous meaning to index-matching circuits, we will need to define the theory of such circuits in a more restrictive way. This is done formally in Appendix A.8; here, we will stress the main features of the theory thus obtained.

The idea is to go in the opposite direction: instead of starting with maps and defining graphs to represent their compositions, we shall start with abstract graphs, then interpret their wires and nodes as spaces and maps (this idea was loosely inspired by the approach developed in Ref. [44] for the formalisation of superpositions of causal order). We thus define indexed open directed acyclic graphs (IODAGs) as abstract open graphs made of nodes and directed wires, with the wires additionally bearing indices, and with an equivalence relation on indices (indicating which ones are 'the same index'). Figure 3.1 shows some examples of IODAGs.

One can, as a second step, *interpret* an IODAG by assigning sectorised Hilbert spaces to wires and maps to nodes, where the maps follow the routes specified by the index-matching in the diagram; this provides an index-matching circuit.[12] This procedure allows us to attribute proper semantics to index-matching quantum circuits.

IODAGs can be composed sequentially and in parallel. To prevent the appearance, in their interpretations, of ambiguities such as the ones described above, the possibility of sequential composition will be restricted: sequentially composing Γ_1 and Γ_2 is allowed only if Γ_1's output wires are the same as Γ_2's input wires, and if the equivalence classes among Γ_1's outputs' indices are the same as those among Γ_2's inputs' indices. For instance, taking the following IODAGs:

$$
\begin{array}{cc}
(e) & (f1) \\
(f2) & (f3)
\end{array}
\tag{3.23}
$$
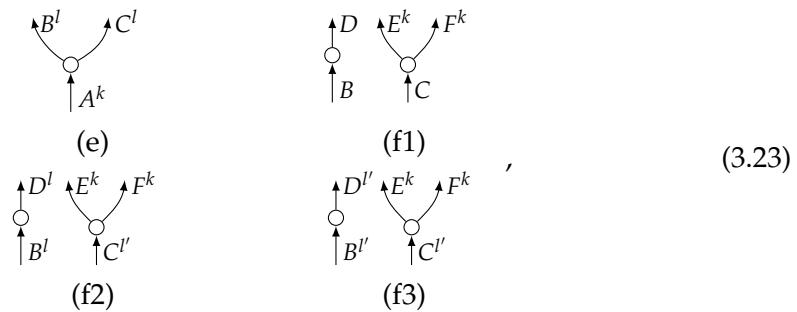
(e) cannot be composed with (f1) or with (f2), but it can be composed with (f3). In a sequential composition, equivalence classes which appear in the interface wires are merged; at the graphical level, this can lead to some relabelling. For instance, the composition of (e) and (f3) defined above yields

$$
\tag{3.24}
$$

Parallel composition, on which there are no restrictions, can lead to some relabelling as well; for instance, the parallel composition of (e) and (f2) is

$$
\tag{3.25}
$$

3.4.3 The validity condition

For index-matching diagrams, the rules for suitable composition of routed isometries (or unitaries) can be superseded by a *global* rule, in which one simply has to consider the graph as a whole to determine whether it yields a valid interpretation. Furthermore, this can be determined via an intuitive and diagrammatic rule.

---

[12] Another way to proceed, more in line with the ideas of Chapter 5, would be to interpret the IODAG as a routed superchannel.

Let us define a 'starting point' for an index as a node that features this index in its outputs but not in its inputs. An IODAG is proper for routed isometries if, for any index appearing in it, there is at most one starting point in the circuit for this index, and no starting point if this index appears in the global input wires of the diagram. It is proper for routed unitaries if it satisfies both this rule and a symmetric one for endpoints. For example, if we consider the diagrams of Figure 3.1, (a), (b) and (c) are suitable for isometries, but not (d), as it features two starting points for the index k. (a) and (b) are also suitable for unitaries, but not (c), as the index k is present in the global outputs of the diagram and has an endpoint.

Finally, as we have said, interpretations of IODAGs are given by assigning sectorised Hilbert spaces to wires and maps to nodes, where the maps follow the routes specified by the index-matching in the diagram. An interpretation of an IODAG thus yields a global index-matching routed map, called the *meaning* of this interpretation. The meaning is obtained by composing the maps for each node in accordance with the graph, then composing with a pre-processing map, which serves to match input indices: the meaning of an interpretation of (f3), for instance, needs to include a pre-processing with a projector which will match the indices of its two input wires. Theorems A.8.6, A.8.7 and A.8.8 in Appendix A.8 ensure that interpreting is a well-defined protocol, playing well with sequential and parallel compositions of IODAGS. Interpreting (a) in routed unitaries, for example, yields a circuit of the form (2.16), which will therefore have a proper and unambiguous signification as a circuit of index-matching routed maps, and whose meaning will automatically be a unitary map. This ensures that our paradigmatic example of an index-matching quantum circuit is completely sound.

IODAGs could be applied to general quantum channels as well; the only difference is that each index will then become a pair of indices, to be able to denote constraints on coherence.

Finally, let us note that index-matching quantum circuits only form a sub-framework of routed quantum circuits. A first example is that a route $\lambda = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$ cannot be written in terms of Kronecker-deltas; thus a routed map with this route would not be describable in the sole framework of index-matching quantum circuits. Another, more physically grounded example is that of the superposition of three trajectories, as depicted in (3.16): it can be shown that (even in the unitary case) the sectorial correlations among the three wires in this diagram cannot be described using only Kronecker deltas.

Chapter 4

An application: coherent control as a task performed on sector-preserving channels

Nothingness was only an idea in my head, an existing idea floating in this immensity: this nothingness had not come before existence, it was an existence like any other and appeared after many others. I shouted 'filth! what rotten filth!'

Jean-Paul Sartre, *Nausea*.

4.1 Introduction

This chapter presents an application of our framework. We show how its conceptual architecture allows us to clarify a long-standing misapprehension of the problem of coherent control that, we argue, was imputable to the inadequacy of standard circuits in this case.

In a sense, the resolution to this issue presented in this chapter will be nothing else than a reiteration of the formalisation of the superposition of trajectories, as presented in Ref. [56] and in Chapter 3. It will thus inevitably involve some redundancy. This is due to the fact that, as we already commented on, the problem of coherent control is an ubiquitous one, that was encountered in the literature from various sides, and consequently, described in various terms. Ref. [56], for instance, studied coherent control for its communicational advantages, and our Chapter 3 restricted itself to discuss its formal aspects. Our goal here is to specifically address the *computational* facet of the problem: how can coherent control be framed as an architecture in a quantum computer or a quantum experiment?

As we shall see, there is a specific history to this computational aspect of coherent control in the literature, one that calls for clear-cut clarification, specifically using the computational vocabulary and directly addressing existing characterisations of the situation. This is what we set ourselves to do here, by bringing in crucial ideas from
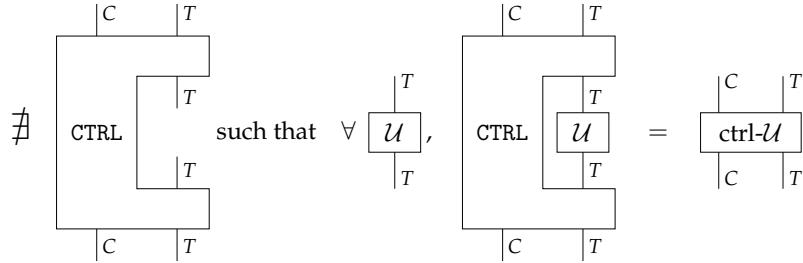
(A) **No-go theorem on coherent control with black box channels** [12, 13, 64, 65, 111, 112]. No superchannel can convert an arbitrary unitary channel $\mathcal{U}$, acting on a target system T, into its controlled version ctrl-$\mathcal{U}$, acting on a control system C and on the target T.
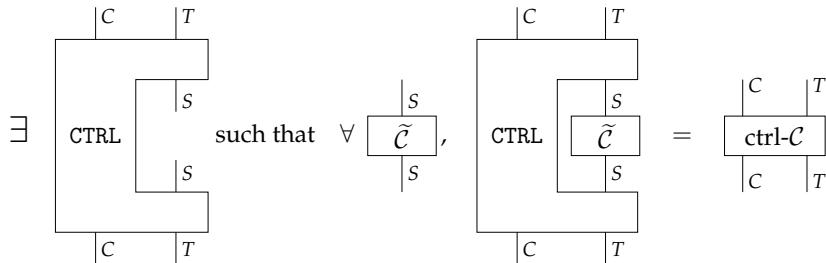
(B) **Universal coherent control with sector-preserving channels.** There exists a superchannel CTRL that transforms arbitrary sector-preserving channels $\widetilde{\mathcal{C}}$ acting on an extended input system S (with Hilbert space $\mathcal{H}_S = \mathbb{C} \oplus \mathcal{H}_T$) into arbitrary controlled channels ctrl-$\mathcal{C}$. In particular, the superchannel CTRL maps arbitrary sector-preserving unitary channels $\widetilde{\mathcal{U}}$ into the corresponding controlled unitary channels ctrl-$\mathcal{U}$.

FIGURE 4.0: Comparison between the standard no-go theorem and our universal controllisation circuit.

routed circuits. This will be an occasion to dive deeper into the technical aspects of a specific application of our framework, as opposed to the more high-level discussion of the rest of this thesis.

Let us first introduce the stakes of the problem of coherent control in quantum computation, and the state of the literature on this subject. A number of quantum algorithms, such as Kitaev's phase estimation algorithm [106] and the DQC1 trace estimation algorithm [107], are based on the use of controlled unitary gates. In computational terms, controlled gates represent a quantum version of the *if-then* clause, in which a subroutine is executed depending on the value of a control variable. In the controlled gate ctrl-U, the quantum state of a control system determines whether or not a target system is subject to a given unitary gate U. When the control system is in a superposition state, the target system experiences a coherent superposition of quantum evolutions [67]. Quantum programming languages that exploit coherent control of quantum gates have been proposed in Refs. [108–110].

The standard way to construct quantum controlled gates is via universal gate sets. To build the controlled gate ctrl-U, one first decomposes the gate U into elementary gates, and then adds control to each of these gates [113]. This construction, however, requires a decomposition of the gate U into elementary gates. In many applications, such as quantum factoring [114], the decomposition is known, because the gate U is the quantum realisation of a classical function, for which a classical

program is given. In other applications, however, the gate U may be completely unknown: in a cloud computing scenario, for example, the gate U may be implemented remotely by a server, and the program that generated U may be unknown to the client. In these situations, it would be convenient to have a way to generate the controlled gate `ctrl`-U from the access to an unknown, uncontrolled gate U. The ability to generate controlled gates would also benefit the implementation of standard quantum algorithms, providing them with an appealing modularity feature [65]. Besides quantum computation, the ability to control an unknown quantum process would be beneficial to other information-processing tasks, such as quantum communication [49, 56, 115], quantum metrology [37, 116], and quantum machine learning [117, 118].

The problem of the coherent control of an unknown channel can be phrased in the following way: 'Is there a universal protocol which, from the use of a black-box channel $\mathcal{C}$, implements its coherently controlled version?'. It has been proven several times, in ever stronger ways [12, 13, 64, 65, 111, 112], that the answer to this question is a resounding 'No': no quantum circuit can 'controllise' arbitrary operations. For generic non-unitary channels, such a controllisation is not even unambiguously defined in the first place, as observed in Ref. [66].

Yet, as has been noted at the same time, coherent control is actually easily implementable in various contexts, such as optical systems [14, 63, 119, 120], trapped ions [63, 120], and superconducting qubits [121]. These realisations are not in contradiction with the no-go theorems because the resources they use are not black boxes: in the computer science terminology, they are grey boxes, whose action is partially known [13, 65] (see also Section 4.3.2 of this chapter for a further elaboration of this point).

This mismatch between theory and experiments suggests that it may be necessary to revisit the terms of the problem. A suitable formulation of the problem would help understanding in which situations, from which resources, and with which protocols, one can implement a coherently controlled quantum channel. This understanding would allow one to go beyond the existing examples of implementations of coherent control, and to compare their respective advantages. Another upshot of a better theoretical understanding is that it allows one to neatly distinguish the informational, implementation-independent aspects of coherent control from the specific, system-dependent features of experimental implementations. In particular, it would help shift the focus away from optical implementations and towards a more implementation-neutral perspective. Finally, identifying the operational ingredients of coherent control helps elucidate some aspects of the existing no-go theorems, as studying protocols that can perform a certain task usually helps understanding why other protocols cannot.

In this chapter we analyse the key features of the experimental implementations, and put forward a new formulation of the problem of coherent control based on

these features. Our starting point is the observation that the crucial feature of the existing implementations is that they use *sector-preserving channels*; i.e., channels whose input systems can be partitioned into sectors (orthogonal subspaces), with the property that a state in a given sector always remains in this sector after the channel has acted. We focus on the case where one sector is one-dimensional and the other is d-dimensional. A sector-preserving channel acting on such a system will be called a *sector-preserving channel of type* $(1, d)$.

The idea of regarding sector-preserving channels as resources originates from Ref. [56], and was further explored in Refs. [49, 115].[1] In these works, the focus was put on the use of sector-preserving channels for communication.[2] In contrast, the relevance of sector-preserving channels to the computational task of coherent control has not been explored before, and will be the focus of this chapter.

Our main results are summarised in the following. For the standard notion of coherent control, we establish a perfect, one-to-one correspondence between sector-preserving channels of type $(1, d)$ and coherently controlled channels with target systems of dimension d. We then show that this one-to-one correspondence can be implemented physically, by inserting sector-preserving channels into a fixed, universal quantum circuit that generates the corresponding controlled channels. Mathematically, this universal circuit can be represented as a *quantum superchannel* [10, 15, 17], that is, a transformation of quantum channels, as introduced in Section 2.4.1. We call this particular superchannel the CTRL superchannel, and show that it is invertible. Its inverse CTRL^{-1} is also a superchannel, corresponding to a universal circuit that transforms controlled channels on d-dimensional systems into sector-preserving channels of type $(1, d)$.

Summarising, coherently controlled channels on d-dimensional systems and sector-preserving channels of type $(1, d)$ are fully equivalent resources, and the interconversion of these resources is implemented by the CTRL superchannel and by its inverse. It is worth contrasting this result with the existing no-go theorems on coherent control: while control cannot be achieved from general channels on d-dimensional systems, it can be achieved from sector-preserving channels of type $(1, d)$. The comparison is illustrated in Figure 4.0.

We also extend our results to the coherent control of N isometric channels, whose input and output spaces can be of different dimensions. As the initial resource, we take N sector-preserving isometric channels of type $(1 \rightarrow 1, d_{\text{in}} \rightarrow d_{\text{out}})$, meaning that *(i)* the input (output) is partitioned into a 1-dimensional sector and a d_{in}-dimensional (d_{out}-dimensional) sector, and *(ii)* states in the 1-dimensional input sector are mapped into states of in the 1-dimensional output sector, while states in the d_{in}-dimensional input sector are mapped into states of in the d_{out}-dimensional output sector. We then show that this resource can be used to construct a channel

---

[1]In the past, a similar approach had independently been explored in Refs. [57, 58]. A different approach, based on the unitary extension of quantum channels, was developed in Refs. [47, 96, 97].

[2]This was part of a wider discussion about the communication advantages of coherent control of causal order [34, 43, 46, 47, 49].

with coherent control between corresponding isometries. We study explicitly the $N = 2$ case, which readily generalises to arbitrary N. Mathematically, we show that there exists an invertible superchannel 2-CTRL that transforms every pair of sector-preserving isometric channels into the corresponding controlled channel.

In the non-isometric case, however, we find that sector-preserving channels of type $(1 \to 1, d_{\text{in}} \to d_{\text{out}})$ are generally not sufficient to achieve all possible controlled channels. Such channels can instead be realised using sector-preserving channels of type $(1 \to 1, d_{\text{in}} \to d_{\text{out}}d')$, where d' is the dimension of an auxiliary system, used to extend the original channels (from a d_{in}-dimensional system to a d_{out}-dimensional system) to isometries. Using this extra resource, we provide a universal protocol for the implementation of coherent control from N sector-preserving channels.

The conceptual connection with the routed circuits of Chapter 3 is obvious; we conclude this chapter by making it formally explicit as well. We do so by introducing 'superchannels on routed channels', i.e. superchannels whose inputs are restricted to be channels that follow prescribed routes. We present the CTRL and 2-CTRL superchannels constructed earlier as superchannels on routed channels; this allows us to write them in a clearer and more concise way – and in particular, as explicitly unitary superchannels.

Our results open the way to two main applications. First, by identifying the resources for the task of coherent control, we lay the basis for a resource-theoretic analysis of existing protocols and experiments. Second, the superchannels defined in this work can be easily extended to multiple channels, and to more elaborate architectures involving multiple instances of coherent control at different moments of time. This flexibility can help the design of complex protocols and algorithms, offering a built-in modularity feature.

The structure of the chapter is as follows. In Section 4.2, we review the existing definitions of controlled unitaries and channels, and we address their extension to multiple channels, defining a new notion of compositely-controlled channels. In Section 4.3, we analyse the structure of the existing implementations of coherent control, and use it to motivate a study of sector-preserving channels of type $(1, d)$. We then show that these channels are in one-to one correspondence with controlled channels on a d-dimensional system. In Section 4.4, we show that the correspondence between sector-preserving channels of type $(1, d)$ and controlled channels can be physically implemented by a universal protocol, formalised by the CTRL superchannel. In Section 4.5, we generalise this correspondence to the coherent control between N isometries, showing that it can also be realised via a universal protocol, and we discuss the case of the coherent control between N general channels, showing that it requires more involved resources. Finally, in Section 4.6 we define superchannels on routed channels, providing a general framework for the manipulation of sector-preserving channels and more general channels that transform sectors in a prescribed way.

4.2 Coherently controlled quantum channels

In this section, we review the existing definitions of coherently controlled unitaries and channels. Then, we provide a one-to-one parametrisation of the possible controlled versions of a channel in terms of a *'pinned Kraus operator'*. Finally, we discuss more general types of controlled quantum channels, and we provide one-to-one parametrisations for these in terms of pinned Kraus operators.

4.2.1 Controlled channels and pinned Kraus operators

Let us start with the most basic definition of controlled operation: controlled unitary gates. Given a unitary operator U acting on a d-dimensional Hilbert space $\mathcal{H}_T$, there is a standard notion of a 'controlled-U' channel: it is the channel corresponding to the unitary operator

$$\texttt{ctrl-}U := |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U \,, \tag{4.1}$$

acting on a composite system, made of a two-dimensional *control* system C and of a d-dimensional *target* system T.

More generally, one may want to control the evolution of an open system. The general evolution of an open system T is described by a quantum channel $\mathcal{C}$, that is, a completely positive, trace-preserving map mapping density matrices on $\mathcal{H}_T$ into density matrices on $\mathcal{H}_T$. The action of the channel $\mathcal{C}$ on a generic density matrix ρ can be conveniently described in the Kraus representation, as $\mathcal{C}(\rho) = \sum_{i=1}^{n} C_i \rho C_i^\dagger$, where the operators $(C_i)_{i=1}^n$, called Kraus operators, satisfy the normalisation condition

$$\sum_{i=1}^{n} C_i^\dagger C_i = I \,, \tag{4.2}$$

I being the identity operator on $\mathcal{H}_T$.

Crucially, the Kraus representation of a channel is not unique: if V is a $l \times n$ isometry with matrix elements V_{ji}, the operators $(C_j')_{j=1}^l$ defined by $C_j' := \sum_i V_{ji} C_i'$ also form a Kraus representation of channel $\mathcal{C}$. The non-uniqueness of the Kraus representation will play an important role in this chapter.

For a general quantum channel $\mathcal{C}$, the definition of coherent control is not straightforward. The naive generalisation of Eq. (4.1) would be to pick a Kraus representation $(C_i)_i$ and define the controlled operators $\texttt{ctrl-}C_i = |0\rangle\langle 0| \otimes C_i + |1\rangle\langle 1| \otimes I$. This definition, however, would fail to give a quantum channel, because the above operators fail to satisfy the normalisation condition (4.2). A suitable generalisation of Eq. (4.1) was put forward in Ref. [66]: a controlled version of channel $\mathcal{C}$ is the channel with Kraus operators

$$\texttt{ctrl}_{\alpha_i}\texttt{-}C_i := \alpha_i |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes C_i \,, \tag{4.3}$$

where $(\alpha_i)_{i=1}^n$ are complex amplitudes satisfying the normalisation condition $\sum_{i=1}^n |\alpha_i|^2 = 1$.

This definition is a special case of the definition of coherent control of two general channels considered in Refs. [47, 56, 57, 68], in the special case where one of the two channels is the identity channel.

It is important to observe that the definition of the controlled channel does not depend only on the channel $\mathcal{C}$. In general, it can depend both on the set of Kraus operators $\mathbf{C} := (C_i)_{i=1}^n$ and on the set of amplitudes $\boldsymbol{\alpha} := (\alpha_i)_{i=1}^n$ used in Eq. (4.3). To emphasise the dependence on the Kraus operators $\mathbf{C}$ and on the amplitudes $\boldsymbol{\alpha}$, we will denote the controlled channel by $\mathtt{ctrl}_{\boldsymbol{\alpha}}^{\mathbf{C}}\text{-}\mathcal{C}$.

Different choices of Kraus operators and amplitudes generally give rise to different versions of controlled channels, with none of these versions being straightforwardly more natural than the other (although some may be more or less coherent [66]). Given that the definition of controlled channels is non-unique, an important question is how to parametrise the possible controlled channels in a compact way. As it turns out, the parametrisation $\mathtt{ctrl}_{\boldsymbol{\alpha}}^{\mathbf{C}}\text{-}\mathcal{C}$ is quite redundant: in fact, many choices of $\mathbf{C}$ and of $\boldsymbol{\alpha}$ give rise to the same controlled channel $\mathtt{ctrl}_{\boldsymbol{\alpha}}^{\mathbf{C}}\text{-}\mathcal{C}$.

In the following, we provide a simple one-to-one parametrisation of the possible controlled channels corresponding to a given uncontrolled channel $\mathcal{C}$: the controlled channels are in one-to-one correspondence with pairs of the form $(\mathcal{C}, C_1)$, where C_1 is a fixed Kraus operator of $\mathcal{C}$. We call the pair $(\mathcal{C}, C_1)$ a *channel with a pinned Kraus operator*.

First, we prove that any controlled version of $\mathcal{C}$ has a Kraus representation in which only the first Kraus operator is coherent with the identity:

Lemma 4.2.1. *For every controlled channel* $\mathtt{ctrl}_{\boldsymbol{\alpha}}^{\mathbf{C}}\text{-}\mathcal{C}$*, one can find a Kraus representation in which one Kraus operator is of the form* $|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes C_1'$ *and all the others are of the form* $|1\rangle\langle 1| \otimes C_j'$*, where* $\mathbf{C}' := (C_j')_{j=1}^n$ *is a suitable Kraus representation of channel* $\mathcal{C}$*. In other words, one has*

$$\mathtt{ctrl}_{\boldsymbol{\alpha}}^{\mathbf{C}}\text{-}\mathcal{C} = \mathtt{ctrl}_{\mathbf{u_n}}^{\mathbf{C}'}\text{-}\mathcal{C}\,, \tag{4.4}$$

where $\mathbf{u}_n$ *is the n-dimensional column vector with a 1 in the first entry, and 0 in the remaining* $n-1$ *entries.*

Proof. As $\boldsymbol{\alpha}$ is a normalised vector in $\mathbb{C}^n$, one can find a unitary matrix V sending it to the basis vector $\mathbf{u}_n$, i.e. $V\boldsymbol{\alpha} = \mathbf{u}_n$. Then, the Kraus operators $(C_j')_{j=1}^n$ defined by $C_j' := \sum_j V_{ji} C_i$ form an alternative Kraus representation of $\mathcal{C}$, and the Kraus operators $(K_j)_{j=1}^n$ defined by $K_j := \sum_j V_{ji}(\mathtt{ctrl}_{\alpha_i}\text{-}C_i)$ form an alternative Kraus representation of $\mathtt{ctrl}_{\boldsymbol{\alpha}}^{\mathbf{C}}\text{-}\mathcal{C}$. It is straightforward to see that $K_1 = \mathtt{ctrl}_1\text{-}C_1'$ and $K_j = \mathtt{ctrl}_0\text{-}C_{j'}$ for every $j > 1$. Hence, $\mathtt{ctrl}_{\boldsymbol{\alpha}}^{\mathbf{C}}\text{-}\mathcal{C}$ can be characterised as in (4.4). □

This result removes the freedom in the choice of the amplitudes $(\alpha_i)_{i=1}^n$: one can simply set the first amplitude to 1, and all the other amplitudes to zero. All

the variability of the controlled channels is then included in the choice of a Kraus representation for channel $\mathcal{C}$.

We now show a further simplification: the definition of the controlled channel depends only on the choice of the *first* Kraus operator in a Kraus representation of $\mathcal{C}$. In other words, the choice of the other Kraus operators does not affect the type of control one obtains.

Lemma 4.2.2. *Let* $\mathbf{C} := (C_i)_{i=1}^m$ *and* $\mathbf{C}' := (C_j')_{j=1}^n$ *be two Kraus representations for channel* $\mathcal{C}$*. Then, the controlled channels* $\mathtt{ctrl}_{\mathbf{u}_m}^{\mathbf{C}}\text{-}\mathcal{C}$ *and* $\mathtt{ctrl}_{\mathbf{u_n}}^{\mathbf{C}'}\text{-}\mathcal{C}$ *coincide if and only if the operators* C_1 *and* C_1' *coincide. In formula,*

$$\mathtt{ctrl}_{\mathbf{u}_m}^{\mathbf{C}}\text{-}\mathcal{C} = \mathtt{ctrl}_{\mathbf{u}_n}^{\mathbf{C}'}\text{-}\mathcal{C} \qquad \Longleftrightarrow \qquad C_1 = C_1'. \tag{4.5}$$

Proof. We start with the direct implication. Without loss of generality, we take $m = n$, as one can always include null Kraus operators and match the cardinality of the Kraus representations of $\mathtt{ctrl}_{\mathbf{u}_m}^{\mathbf{C}}\text{-}\mathcal{C}$ and $\mathtt{ctrl}_{\mathbf{u}_n}^{\mathbf{C}'}\text{-}\mathcal{C}$. If the two controlled channels coincide, then there exists a unitary matrix W that connects their Kraus representations. In particular, one must have

$$C_1 \otimes |1\rangle\langle 1| + I \otimes |0\rangle\langle 0| = W_{11} \left(C_1' \otimes |1\rangle\langle 1| + I \otimes |0\rangle\langle 0| \right) + \sum_{j>1} W_{1j} C_j' \otimes |1\rangle\langle 1|.$$

$$\tag{4.6}$$

Taking the expectation value on the vector $|0\rangle$ on both sides of the equation, we then obtain the relation $I = W_{11} I$, which implies $W_{11} = 1$, and, since W is a unitary matrix, $W_{1j} = 0$ for every $j > 1$. Inserting this condition in Eq. (4.6) we obtain $C_1 = C_1'$.

For the converse implication, suppose that $C_1 = C_1'$. Then, for an arbitrary product state $\rho_C \otimes \rho_T$ of the control and the target, we have

$$\begin{aligned}
\mathtt{ctrl}_{\mathbf{u}_m}^{\mathbf{C}}\text{-}\mathcal{C}(\rho_C \otimes \rho_T) &= \mathtt{ctrl}_1\text{-}C_1 \left(\rho_C \otimes \rho_T \right) (\mathtt{ctrl}_1\text{-}C_1)^\dagger + \sum_{i>1} \mathtt{ctrl}_0\text{-}C_i \left(\rho_C \otimes \rho_T \right) (\mathtt{ctrl}_0\text{-}C_i)^\dagger \\
&= \mathtt{ctrl}_1\text{-}C_1 \left(\rho_C \otimes \rho_T \right) (\mathtt{ctrl}_1\text{-}C_1)^\dagger + |0\rangle\langle 0|\rho_C|0\rangle\langle 0| \otimes \left(\mathcal{C}(\rho_T) - C_1 \rho_T C_1^\dagger \right) \\
&= \mathtt{ctrl}_1\text{-}C_1' \left(\rho_C \otimes \rho_T \right) (\mathtt{ctrl}_1\text{-}C_1')^\dagger + |0\rangle\langle 0| \otimes \rho_C|0\rangle\langle 0| \left(\mathcal{C}(\rho_T) - C_1' \rho_T C_1'^\dagger \right) \\
&= \mathtt{ctrl}_1\text{-}C_1' \left(\rho_C \otimes \rho_T \right) (\mathtt{ctrl}_1\text{-}C_1')^\dagger + \sum_{j>1} \mathtt{ctrl}_0\text{-}C_j' \left(\rho_C \otimes \rho_T \right) \left(\mathtt{ctrl}_0\text{-}C_j' \right)^\dagger \\
&= \mathtt{ctrl}_{\mathbf{u}_n}^{\mathbf{C}'}\text{-}\mathcal{C}(\rho_C \otimes \rho_T).
\end{aligned} \tag{4.7}$$

Since ρ_C and ρ_T are arbitrary, we conclude $\mathtt{ctrl}_{\mathbf{u}_m}^{\mathbf{C}}\text{-}\mathcal{C} = \mathtt{ctrl}_{\mathbf{u}_n}^{\mathbf{C}'}\text{-}\mathcal{C}$. $\qquad\square$

Combining Lemmas 4.2.1 and 4.2.2, we obtain a non-redundant parametrisation of the possible controlled versions of a given channel:

Theorem 4.2.1. *The controlled versions of channel $\mathcal{C}$, as defined by Eq. (4.3), are in one-to-one correspondence with the possible choices of a single Kraus operator for channel $\mathcal{C}$.*

By 'a Kraus operator for channel $\mathcal{C}$', we mean a Kraus operator appearing in at least one Kraus representation for $\mathcal{C}$. Equivalently, the possible Kraus operators for a given channel can be characterised as follows:

Lemma 4.2.3. *An operator C_1 is a Kraus operator for channel $\mathcal{C}$ if and only if the map $\mathcal{C}_- : \rho \mapsto \mathcal{C}(\rho) - C_1 \rho C_1^\dagger$ is completely positive.*

Proof. The 'only if' part is immediate. For the 'if' part, a Kraus representation for $\mathcal{C}$ containing the operator C_1 can be built by picking an arbitrary Kraus representation for the map $\mathcal{C}_-$, say $(C_i)_{i=2}^n$. For any such choice, the operators $(C_i)_{i=1}^n$ form a Kraus representation for channel $\mathcal{C}$. $\qquad\square$

Hereafter, we will call the single Kraus operator picked in Theorem 4.2.1 a *pinned Kraus operator*. A channel with a pinned Kraus operator will be represented by the pair $(\mathcal{C}, C_1)$. Given a pinned Kraus operator C_1, and an arbitrary completion of it into a Kraus representation $(C_i)_i$, the corresponding controlled version of $\mathcal{C}$ is given by the Kraus operators

$$\begin{cases} \widehat{C}_1 = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes C_1 \\ \widehat{C}_i = |1\rangle\langle 1| \otimes C_i \qquad \forall i \geq 2 \,. \end{cases} \tag{4.8}$$

From now on, we will use the notation $\mathtt{ctrl}_{C_1}\text{-}\mathcal{C}$ to denote the controlled channel with the above Kraus operators. The action of the controlled channel $\mathtt{ctrl}_{C_1}\text{-}\mathcal{C}$ on a generic product state of the target system and of the control is

$$\begin{aligned} \mathtt{ctrl}_{C_1}\text{-}\mathcal{C}(\rho_C \otimes \rho_T) &= \sum_i \widehat{C}_i \, (\rho_C \otimes \rho_T) \, \widehat{C}_i^\dagger \\ &= \langle 0|\rho_C|0\rangle \; |0\rangle\langle 0|_C \otimes \; \rho_T \\ &\quad + \langle 1|\rho_C|1\rangle \; |1\rangle\langle 1|_C \otimes \; \mathcal{C}(\rho_T) \\ &\quad + \langle 1|\rho_C|0\rangle \; |1\rangle\langle 0|_C \otimes \; C_1 \, \rho_T + \text{h.c.} \,, \end{aligned} \tag{4.9}$$

where h.c. denotes the Hermitian conjugate. In the above formula, the first two terms in the sum represent the classical control on the channel, while the second two terms represent the 'coherent part' of the controlled operation.

This pinned Kraus operator C_1 coincides with the 'transformation matrix' of Ref. [47], the 'vacuum interference operator' of Ref. [56], and the 'K operator' of Ref. [66]. Ref. [47] derived the 'transformation matrix' from a Stinespring dilation of the channel $\mathcal{C}$, and interpreted it as the additional information that has to be provided about the physical implementation of channel $\mathcal{C}$ in order to build a controlled channel. In contrast, Ref. [56] derived the 'vacuum interference operator' from an extension of channel $\mathcal{C}$ to a larger channel that can act also on the vacuum. In this

chapter, we will make connection with the latter approach, showing that the controlled channel $\mathtt{ctrl}_{C_1}\text{-}\mathcal{C}$ is in one-to-one correspondence, both mathematically and physically, with a particular extension of the original channel $\mathcal{C}$, corresponding to the vacuum extension of Ref. [56].

Compared to Refs. [47, 56, 66], our presentation makes it evident that the operator characterising a controlled version of channel $\mathcal{C}$ can be simply understood as a Kraus operator of this channel, a fact that has not been pointed out before.[3] In addition, the explicit relation between control and pinned Kraus operators suggests further extensions of the notion of quantum control, as discussed in the next subsection.

4.2.2   Control between multiple noisy channels

We now consider a generalisation of the notion of coherent control: the case in which each of the two values of the control is associated to the execution of a different channel on the target system. In other words, we now consider the coherent control between the execution of two channels $\mathcal{A}$ and $\mathcal{B}$, rather than between one channel and the identity channel. We will now take the input and output target systems, T_{in} and T_{out}, to be of possibly different dimensions.

Before entering into the technical details, it may be helpful to note that different authors have used different names for what is essentially the same notion: Refs. [67], [68], [57], [47], [56] use the expressions 'superposition of time evolutions', 'interference of CP maps', 'gluing of CP maps', 'coherent control of quantum channels', and 'superposition of quantum channels', respectively. We review the existing terminologies in Appendix B.1.

If we start with the basic case of two isometric gates, represented by two isometries $U, V : \mathcal{H}_{T_{\text{in}}} \rightarrow \mathcal{H}_{T_{\text{out}}}$, the standard notion of a 'controlled-(U, V)' channel is given by the isometry

$$\mathtt{ctrl}\text{-}(U, V) := |0\rangle\langle 0| \otimes U + |1\rangle\langle 1| \otimes V. \tag{4.10}$$

Extending this definition to the case of the control between two noisy evolutions, represented by CPTP maps $\mathcal{A}, \mathcal{B} : \mathcal{L}(\mathcal{H}_{T_{\text{in}}}) \rightarrow \mathcal{L}(\mathcal{H}_{T_{\text{out}}})$, requires more work. Once again, there are a variety of ways of defining the controlled version of $\mathcal{A}$ and $\mathcal{B}$. These different versions can be obtained by picking Kraus representations of same length[4] $(A_i)_{i=1}^n$ and $(B_i)_{i=1}^n$ for $\mathcal{A}$ and $\mathcal{B}$ and defining the Kraus operators:

$$\mathtt{ctrl}\text{-}(A_i, B_i) := |0\rangle\langle 0| \otimes A_i + |1\rangle\langle 1| \otimes B_i. \tag{4.11}$$

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[3]A proof in Ref. [66] mentioned that any possible 'K operator' is a Kraus operator of $\mathcal{C}$, without however discussing the reverse implication.

[4]Note that any two Kraus representations can be taken to be of the same length by adjoining 0's to the shortest one.

A one-to-one parametrisation of the possible choices is provided in the following theorem, proven in Appendix B.2:

Theorem 4.2.2. *Given a Kraus representation* $(A_i)_{i=1}^n$ *of minimal length of* $\mathcal{A}$*, the choice of a control between* $\mathcal{A}$ *and* $\mathcal{B}$ *is in one-to-one correspondence with the choice of n Kraus operators of* $\mathcal{B}$*.*

By 'n Kraus operators of $\mathcal{B}$', we mean n operators that appear together in at least one Kraus representation of $\mathcal{B}$. Calling these operators B_i's, and arbitrarily completing them into a Kraus representation $(B_i)_{i=1}^{n'}$ of $\mathcal{B}$, Kraus operators for the corresponding controlled channel are given by the concatenation of the $(\texttt{ctrl-}(A_i, B_i))_{i=1}^n$ and the $(\texttt{ctrl-}(0, B_i))_{n < i \leq n'}$. Note that in this parametrisation, only the Kraus operators of $\mathcal{B}$ vary; those of $\mathcal{A}$ are fixed from the start.

The previous considerations can be extended to the case of a control system of dimension N, controlling between the execution of N channels $\mathcal{C}^1, \ldots, \mathcal{C}^N$. A strategy would be to proceed via recursion, first picking a control between $\mathcal{C}^1$ and $\mathcal{C}^2$, then picking a control between this controlled channel and $\mathcal{C}^3$, etc.

4.3 A new resource for coherent control: sector-preserving channels

Here we discuss the physical resources needed to implement coherent control of general quantum channels.

4.3.1 A no-go theorem for coherent control of unitary gates, and a way to evade it

It has been proven in various ways that it is impossible to construct a controlled unitary gate starting from a black box that implements the corresponding uncontrolled unitary gate [12, 13, 64, 65, 111, 112]. Mathematically, the no-go theorem is that it is impossible to find a quantum superchannel that transforms a generic unitary channel $\mathcal{U} : \rho \mapsto U\rho U^\dagger$ into the controlled unitary channel $\texttt{ctrl-}\mathcal{U} : \rho \mapsto \texttt{ctrl-}U \rho \, \texttt{ctrl-}U^\dagger$ with the operator $\texttt{ctrl-}U$ defined in Eq. (4.1).

The origin of the impossibility is that the uncontrolled unitary channel $\mathcal{U}$ is provided as a *black box*, without any further information on its action except for the fact that $\mathcal{U}$ is known to be unitary. One way to evade the no-go theorem is to start from a device that is not a complete black box, but rather a *grey box*, whose action is partially known. For example, one could be given a device that implements a unitary gate $\widetilde{U} = |\phi_0\rangle\langle\phi_0| \oplus U$, where $\widetilde{U}$ acts on $\mathcal{H}$ and U is an unknown unitary gate acting on a d-dimensional sector (i.e. orthogonal subspace) $\mathcal{H}^1 \subseteq \mathcal{H}$, and $|\phi_0\rangle$ is another state, orthogonal to all the states in $\mathcal{H}^1$. In this case, the action of the device in the sector $\mathcal{H}^1$ is unknown, while the action of the device on the vector $|\phi_0\rangle$ is known. In

this setting, the controlled gate `ctrl`-U can be built from the gate $\widetilde{U}$ using a simple quantum circuit [13, 63, 65].

The use of grey boxes that act in a known way on some input states is central to all existing proposals for experimental implementations of coherent controls of unitary gates. For example, photonic implementations [14, 119] achieve coherent control of certain optical devices, such as polarisation rotators, by exploiting the fact that such devices are passive, and therefore transform the vacuum state into itself. In these examples, the sector $\mathcal{H}^1$ is spanned by single-photon polarisation states, and the state $|\phi_0\rangle$ is the zero-photon Fock state.

In trapped-ions implementations [63, 120], the input device uses a laser pulse to implement a unitary gate by stimulating the transition between the two electronic levels. The pulse is far off resonance with the transition between the other electronic levels of the ion, and therefore the device acts trivially on such levels. In this case, the state $|\phi_0\rangle$ can be any of the levels that are unaffected by the pulse. A similar situation arises in superconducting-qubits implementations [121].

In summary, all the existing proposals of experimental implementations use grey box unitary gates $\widetilde{U}$ that act

1. as unknown gates U on a sector $\mathcal{H}^1 \simeq \mathcal{H}_T$, and

2. as the identity gate I on another sector $\mathcal{H}^0$, orthogonal to $\mathcal{H}^1$.

In the following we will extend this scheme from unitary gates to arbitrary noisy channels, and to the case of gates acting as the identity on several sectors, showing that access to a suitable grey box channel allows one to build a controlled channel that is in one-to-one correspondence with it.

We will restrict ourselves to the case in which the sectors on which the identity is applied are one-dimensional; however, all our arguments could be extended to the case in which they are multi-dimensional and the grey boxes act as the identity on each of them. Note that when the extension sectors have the same dimension as $\mathcal{H}^0$, the above requirements lead to the usual definition of controlled channels.

4.3.2 Modelling noisy grey boxes: sector-preserving channels

We now consider how the grey box approach of the previous section can be extended from unitary gates to arbitrary noisy channels. As we will see – and as the reader might have guessed at this point –, this amounts precisely to a study of sectorial constraints, for which the routed circuits of Chapter 3 provide the relevant formalisation.

We consider a noisy quantum channel $\widetilde{\mathcal{C}}$ that acts on a system S with a Hilbert space $\mathcal{H}_S$ partitioned into two sectors, $\mathcal{H}_S = \mathcal{H}_S^0 \oplus \mathcal{H}_S^1$, with $\mathcal{H}_S^0$ one-dimensional and $\mathcal{H}_S^1 \simeq \mathcal{H}_T$. The channel $\widetilde{\mathcal{C}}$ will act

1. as a completely unknown channel $\mathcal{C} : \mathcal{L}(\mathcal{H}_S^1) \to \mathcal{L}(\mathcal{H}_S^1)$ on the input states in $\mathcal{L}(\mathcal{H}_S^1)$, and

2. as the identity channel I on the unique input state in $\mathcal{L}(\mathcal{H}_S^0)$.

Such grey boxes have a simple characterisation: they are the sector-preserving channels on $\mathcal{H}_S$.[5]

Definition 4.3.1. *Let* $\mathcal{H}_S = \bigoplus_{k=0}^m \mathcal{H}_S^k$ *be a Hilbert space with a preferred partition into sectors. A channel* $\widetilde{\mathcal{C}} : \mathcal{L}(\mathcal{H}_S) \to \mathcal{L}(\mathcal{H}_S)$ *is* sector-preserving *if it follows a δ route.*[6]

As we saw in Section 3.3.1, there are several possible characterisations of that fact. One is that

$$\forall \rho, \widetilde{\mathcal{C}}(\rho) = \sum_{k,l} \pi^l \circ \widetilde{\mathcal{C}}\left(\pi^l \circ \rho \circ \pi^k\right) \circ \pi^k, \tag{4.12}$$

which can be checked to be equivalent to the condition that $\widetilde{\mathcal{C}}$ preserves the set of states with support in the subspace $\mathcal{H}_S^k$, for every $k \in \{0, \dots, m\}$:

$$\forall k, \forall \rho \in \mathcal{L}(\mathcal{H}_S^k), \quad \mathcal{C}(\rho) \in \mathcal{L}(\mathcal{H}_S^k). \tag{4.13}$$

Note that $\rho \in \mathcal{L}(\mathcal{H}_S^k)$ equivalently means that $\mathsf{Supp}(\rho) \subseteq \mathcal{H}_S^k$, where $\mathsf{Supp}(\rho)$ denotes the support of ρ. The condition (4.13) was called the 'no-leakage condition' in Ref. [56].

Finally, from Theorem 3.3.3, we know that, picking an arbitrary Kraus representation $(\widetilde{C}_i)_i$ of $\widetilde{\mathcal{C}}$, another equivalent definition of sector-preservingness is that each $\widetilde{C}_i$ follows the route δ, i.e. satisfies

$$\widetilde{C}_i = \sum_k \pi^k \circ \widetilde{C}_i \circ \pi^k. \tag{4.14}$$

When some of the sectors $\mathcal{H}_S^k$ are one-dimensional, the condition of sector preservation (4.13) implies that the channel $\widetilde{\mathcal{C}}$ acts as the identity channel on each of them. In the following, we will denote the sector preserving channels with $\mathrm{dim}(\mathcal{H}_S^k) = 1 \, \forall k < m$ and $\mathrm{dim}(\mathcal{H}_S^m) = d$ as *sector-preserving channels of type* $(\underbrace{1, \dots, 1}_{m \text{ times}}, d)$. In particular, the channels we are considering here are the sector-preserving channels of type $(1, d)$.

The approach of considering an extended channel that acts as $\mathcal{C}$ on a given sector was introduced in Ref. [56]; we reviewed it in Section 2.2.1. There, there was only one one-dimensional sector, which was called the 'vacuum sector', and the channel $\widetilde{\mathcal{C}}$ was called a 'vacuum extension', with this terminology motivated by the photonic implementations. Here, however, we prefer to use the expressions 'extension sectors' and 'extended channel', which are neutral with respect to the choice of experimental implementations.

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[5]We note that the notion of sector-preservingness has been independently introduced in the past, under the name 'subspace-preservingness'; see Ref. [57].

[6]As we are not interested in coherence constraints here, we will be using the lighter notations introduced in Section 3.3.6.

The key point of our approach is that the grey box channel $\widetilde{\mathcal{C}}$, and not the black box channel $\mathcal{C}$, should be regarded as the initial resource for the implementation of coherent control. In other words, we argue that one should shift the terms of the problem away from the question 'what can one do with an unknown channel $\mathcal{C}$?'. Instead, one should ask the question 'what can one do with a channel $\widetilde{\mathcal{C}}$ that acts as an unknown channel on a given sector?'.

A similar shift of perspective was proposed in Refs. [49, 56, 115] for the purpose of defining quantum communication protocols where messages can travel in a coherent superposition of multiple trajectories. In this context, extended channels were used to describe communication devices that can take as input either one particle (corresponding, in our notations, to the sector $\mathcal{H}_S^1$) or the vacuum (corresponding to the sector $\mathcal{H}_S^0$). This modelling was essential to define resource theories of quantum communication [49], where the initial resources are communication devices that can be connected in a coherent superposition of multiple configurations. The present chapter can be viewed as an application of the same approach to the task of the coherent control of quantum channels: the extended channel represents the initial resource, and the question is which types of controlled channel can be constructed from such resource.

4.3.3 The case of one extension sector

The case where there is only one extension sector $\mathcal{H}_S^1$ (i.e., of sector-preserving channels of type $(1, d)$) is particularly relevant in this chapter, because, as we will show later, it provides the fundamental resource for the realisation of the controlled channels defined in Eq. (4.3). We will start by characterising these channels, and show that their characterisation is indeed in full correspondence with that of controlled channels.

In terms of Kraus representation, applying (4.14) yields that the sector-preserving channels of type $(1, d)$ can be characterised as the channels with Kraus operators of the form

$$\widetilde{C}_i = \alpha_i \oplus C_i, \tag{4.15}$$

where $(C_i)_i$ is a Kraus representation of some channel acting on sector $\mathcal{H}_S^1 \simeq \mathcal{H}_T$, and the α_i's are amplitudes satisfying the normalisation condition $\sum_i |\alpha_i|^2 = 1$.

A one-to-one parametrisation of the sector-preserving channels of type $(1, d)$ can be obtained with the same approach as in Section 4.2.

Lemma 4.3.1. *Every sector-preserving channel of type $(1, d)$ has a Kraus representation of the form*

$$\begin{cases} \widetilde{C}_1 = 1 \oplus C_1 \\ \widetilde{C}_i = 0 \oplus C_i \qquad \forall i \geq 2 \,, \end{cases} \tag{4.16}$$

where $(C_i)_i$ is a Kraus representation of some channel on the d-dimensional sector.

Proof. As in the proof of Lemma 4.2.1, this alternative Kraus representation can be found by using a unitary matrix $(V_{ji})_{ji}$ that sends the normalised vector $(\alpha_i)_i$ to $(1, 0, \ldots, 0)$. □

Using the same arguments as in Section 4.2, it is easy to see that the sector-preserving channels $\widetilde{\mathcal{C}}$ are in one-to-one correspondence with pairs $(\mathcal{C}, C_1)$, consisting of a channel acting on sector $\mathcal{L}(\mathcal{H}_S^1)$, and of a Kraus operator for $\mathcal{C}$. In short, we have the following.

Theorem 4.3.1. *The sector-preserving channels of type $(1, d)$ are in one-to-one correspondence with channels with a pinned Kraus operator on their d-dimensional sector.*

The sector-preserving channel of type $(1, d)$ that corresponds to the channel $\mathcal{C}$ with the pinned Kraus operator C_1 on its d-dimensional sector shall be called $\widetilde{\mathcal{C}}[C_1]$. In the case of unitary channels, the characterisation is particularly simple.

Corollary 4.3.1. *Sector-preserving unitary channels of type $(1, d)$ are in one-to-one correspondence with unitary operators in dimension d. Explicitly, the correspondence between sector-preserving unitary channels $\widetilde{\mathcal{U}}$ and unitary operators U is given by the relation*

$$\widetilde{\mathcal{U}}(\rho) = (1 \oplus U) \, \rho \, (1 \oplus U)^\dagger \qquad \forall \rho \in \mathcal{L}(\mathcal{H}_S). \tag{4.17}$$

This is in contrast with the general situation for unitary channels, which correspond to unitary operators only up to an arbitrary global phase. The crucial fact here is that the one-dimensional extension sector can be used to fix this phase gauge in the d-dimensional sector.

Going back to the case of general channels, Theorem 4.3.1 establishes a one-to-one correspondence between sector-preserving channels of type $(1, d)$ and controlled channels:

Corollary 4.3.2. *For any d, the following sets are in one-to-one correspondence:*

1. *controlled channels as defined in (4.3), with a d-dimensional target system;*

2. *sector-preserving channels of type $(1, d)$;*

3. *channels with a pinned Kraus operator in dimension d.*

Let us comment on the respective roles, for our purposes, of the three notions which Corollary 4.3.2 shows to be mathematically equivalent. The first (controlled channels) is essentially an informational notion, with practical use in quantum protocols: this is typically what one wants to eventually obtain. The second (sector-preserving channels of type $(1, d)$) can be understood as the physical resource (with the sector-preserving property often corresponding to physical features of an interaction, such as conservation laws) allowing us to implement the first one. Finally, the third (channels with a pinned Kraus operator) is a purely mathematical notion,
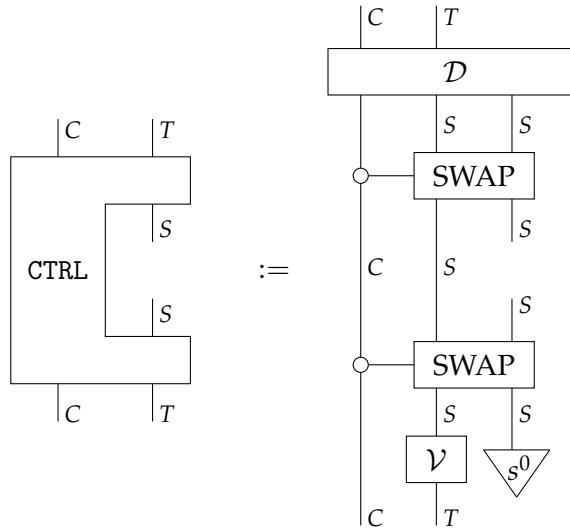
FIGURE 4.1: Quantum circuit for the CTRL superchannel. The superchannel transforms sector-preserving channels acting on a system S with Hilbert space $\mathcal{H}_S = \mathcal{H}_S^0 \oplus \mathcal{H}_S^1$ into controlled channels acting on the composite system $C \otimes T$, consisting of a control system C and of a target system T with Hilbert space $\mathcal{H}_T \simeq \mathcal{H}_S^1$. The sector-preserving channel in input is inserted between two controlled SWAP operations, which in turn are placed between two quantum channels $\mathcal{V}$ and $\mathcal{D}$, which serve as 'adaptors', between the systems T and S, and between the systems $C \otimes S \otimes S$ and $C \otimes T$, respectively.

with no direct practical interpretation, which serves to provide a simple one-to-one mathematical parametrisation to the first two.

In fact, a more careful inspection also reveals that the one-to-one correspondence between the above sets can be implemented by linear maps. For the sets of controlled channels and sector-preserving channels, the correspondence can be implemented physically by quantum circuits that convert sector-preserving channels into controlled channels, and vice-versa. This physical correspondence is the object of the next section.

4.4 The control superchannel and the equivalence between sector-preserving and controlled channels

4.4.1 The control superchannel

In the previous section, we showed that the controlled channels on target systems of dimension d (the $\texttt{ctrl}_{C_1}\text{-}\mathcal{C}$) are in one-to-one correspondence with sector-preserving channels of type $(1, d)$ (the $\widetilde{\mathcal{C}}[C_1]$).

Our point is now to show that for any given d, there is a universal circuit architecture in which an agent who possesses the sector-preserving channel $\widetilde{\mathcal{C}}[C_1]$ can insert this channel in order to implement the controlled channel $\texttt{ctrl}_{C_1}\text{-}\mathcal{C}$.

We thus introduce the *control superchannel*, a superchannel that takes as input any sector-preserving channel $\widetilde{\mathcal{C}}[C_1]$ of type $(1, d)$, and yields the controlled channel $\mathtt{ctrl}_{C_1}\text{-}\mathcal{C}$ acting on a target system of dimension d.

Theorem 4.4.1. *Let $\mathcal{H}_S = \mathcal{H}_S^0 \oplus \mathcal{H}_S^1$ be a Hilbert space, with $\dim(\mathcal{H}_S^0) = 1$ and $\dim(\mathcal{H}_S^1) = d$, let $\mathcal{H}_C$ be a control space of dimension 2, and $\mathcal{H}_T$ be a target space, with $\mathcal{H}_T \simeq \mathcal{H}_S^1$.*

There exists a superchannel $\mathtt{CTRL}$ of type $(S \to S) \to (C \otimes T \to C \otimes T)$ such that for any sector-preserving channel $\widetilde{\mathcal{C}}[C_1]$,

$$\mathtt{CTRL}\left[\widetilde{\mathcal{C}}[C_1]\right] = \mathtt{ctrl}_{C_1}\text{-}\mathcal{C}. \tag{4.18}$$

Furthermore, this superchannel is unitary-preserving on the sector-preserving channels on S.

Proof. Let $V : \mathcal{H}_T \to \mathcal{H}_S$ be the isometry that maps $\mathcal{H}_T$ into the subspace $\mathcal{H}_S^1 \simeq \mathcal{H}_T$, let $|s^0\rangle$ be a unit vector in $\mathcal{H}_S^0$, let $W : \mathcal{H}_C \otimes \mathcal{H}_S \otimes \mathcal{H}_S \to \mathcal{H}_C \otimes \mathcal{H}_T$ be the coisometry defined by $W := I \otimes V^\dagger \otimes \langle s^0|$, and let $\mathcal{D}$ be the quantum channel defined by $\mathcal{D}(\rho) := W\rho W^\dagger + \rho_0 \operatorname{Tr}[P\rho]$, where ρ_0 is a fixed density matrix on $\mathcal{H}_C \otimes H_T$ and $P := I - W^\dagger W$.[7] We then define the superchannel $\mathtt{CTRL}$ through its action on a generic linear map $\mathcal{M} : \mathcal{L}(\mathcal{H}_C \otimes \mathcal{H}_T) \to \mathcal{L}(\mathcal{H}_C \otimes \mathcal{H}_T)$:

$$\mathtt{CTRL}(\mathcal{M}) := \mathcal{D} \circ \mathtt{ctrl}\text{-}\mathcal{SWAP} \circ (\mathcal{I}_C \otimes \mathcal{I}_S \otimes \mathcal{M}) \circ \mathtt{ctrl}\text{-}\mathcal{SWAP} \circ (\mathcal{I}_C \otimes \mathcal{V} \otimes |s^0\rangle\langle s^0|) \tag{4.19}$$

where $\mathcal{V}$ is the quantum channel corresponding to the isometry V, and $\mathtt{ctrl}\text{-}\mathcal{SWAP}$ is the unitary channel corresponding to the controlled SWAP operator (see Figure 4.1 for an illustration).

With this definition, one can verify that the condition $\mathtt{CTRL}[\widetilde{\mathcal{C}}[C_1]] = \mathtt{ctrl}_{C_1}\text{-}\mathcal{C}$ holds. Let us prove it by showing that they act in the same way on pure states, using a Kraus representation for the channel $\widetilde{\mathcal{C}}[C_1]$ with Kraus operators $\widetilde{C}_i = \delta_{i1} \oplus C_i$. From there, it can then be deduced by linearity that the two channels act in the same way on any density matrix, and therefore that they are equal. We take a strict equality $T = S^1$ to avoid unnecessary clutter.

Taking an arbitrary state $|\psi\rangle_{CT}$, we obtain

$$\mathtt{ctrl\text{-}SWAP}(V \otimes |s^0\rangle)\,|\psi\rangle_{CT} = |0\rangle_C \otimes {}_C\langle 0|\psi\rangle_{CS} \otimes |s^0\rangle_S + |1\rangle_C \otimes |s^0\rangle_S \otimes {}_C\langle 1|\psi\rangle_{CS} \tag{4.20}$$

and thus

---

[7]Note that the only thing that matters is how $\mathcal{D}$ acts on the sector $\mathcal{H}_C \otimes \mathcal{H}_S^1 \otimes \mathcal{H}_S^0$ of its input; its action on other sectors is irrelevant and can be defined in an arbitrary way, as long as it gives a CPTP map. This irrelevant part of the action disappears in the formulation as a routed superchannel (Figure 4.5).

$$|\psi_i\rangle := \texttt{ctrl-SWAP}\,(I_C \otimes I_S \otimes \widetilde{C}_i)\,\texttt{ctrl-SWAP}(V \otimes |s^0\rangle))\,|\psi\rangle_{CT}$$

$$= \texttt{ctrl-SWAP}\,\big(\delta_{i1}\,|0\rangle_C \otimes {}_C\langle 0|\psi\rangle_{CS} \otimes |s^0\rangle_S + |1\rangle_C \otimes |s^0\rangle_S \otimes C_i\,{}_C\langle 1|\psi\rangle_{CS}\,\big)$$

$$= \big(\delta_{i1}\,|0\rangle_C \otimes \langle 0|\psi\rangle_{CS} + C_i\,|1\rangle_C \otimes \langle 1|\psi\rangle_{CS}\,\big) \otimes |s^0\rangle\,. \tag{4.21}$$

Now, one has $P\,|\psi_i\rangle = 0$, and $W\,|\psi_i\rangle = \delta_{i1}\,|0\rangle \otimes {}_C\langle 0|\psi\rangle_{CS} + |1\rangle_C \otimes C_i\,{}_C\langle 1|\psi\rangle_{CS} \equiv \texttt{ctrl}_{\delta_{i1}}\text{-}C_i\,|\psi\rangle_{CT}$. Summarising, if the control and target start off in the state $|\psi\rangle_{CT}$, and if the subprocess corresponding to the Kraus operator $\widetilde{C}_i$ takes place, then the final (subnormalized) state is $W|\psi_i\rangle = \texttt{ctrl}_{\delta_{i1}}\text{-}C_i\,|\psi\rangle_{CT}$. On average over all possible values of i, we obtain the evolution

$$\texttt{CTRL}(\widetilde{\mathcal{C}}[C_1])(|\psi\rangle\,\langle\psi|) = \sum_i W|\psi_i\rangle\langle\psi_i|W^\dagger$$

$$= \sum_i (\texttt{ctrl}_{\delta_{i1}}\text{-}C_i)\,|\psi\rangle\,\langle\psi|\,(\texttt{ctrl}_{\delta_{i1}}\text{-}C_i)^\dagger$$

$$= \texttt{ctrl}_{C_1}\text{-}\mathcal{C}(|\psi\rangle\,\langle\psi|)\,.$$

As for the preservation of unitarity on sector-preserving channels, it is sufficient to recall Corollary 4.3.1: unitary sector-preserving channels of type $(1, d)$ are of the form $\widetilde{\mathcal{U}} : \rho \mapsto (1 \oplus U)\rho(1 \oplus U)^\dagger$. By the previous calculation, one then has $\texttt{CTRL}(\widetilde{\mathcal{U}}) : \rho \mapsto (|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U)\rho(|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U)^\dagger$, which is a unitary channel.

$\square$

The superchannel $\texttt{CTRL}$ constitutes a rigorous theoretical formalisation of the existing experimental schemes for the implementation of coherent control. It is the universal protocol through which sector-preserving channels of type $(1, d)$ can be turned into their corresponding controlled channel.

We note that even though we defined this superchannel as accepting as input *any* possible channel $S \to S$, the only thing we are interested in is in fact its action on *sector-preserving* channels. An alternative way of defining it would be to formally restrict its inputs to be only sector-preserving channels (or extensions of those); this would make clearer the fact that this protocol is only useful when sector-preserving channels are used, and would also allow us to get rid of superfluous information in the specification of the superchannel – namely, information that only modifies the action of the superchannel on non-sector-preserving channels. It would also allow us to present the protocols in an explicitly unitary way. We will do this in Section 4.6, coining the notion of *superchannels on routed channels*.

Let us also comment on the specific case of unitary channels. Per Corollary 4.3.1, we know that sector-preserving unitary *channels* of type $(1, d)$ are in one-to-one correspondence with unitary *operators* on their d-dimensional sector. Noting as U the unitary operator corresponding to the unitary sector-preserving channel $\widetilde{\mathcal{U}}$, the control superchannel will then precisely map any sector-preserving unitary channel $\widetilde{\mathcal{U}}$ to the gate applying the controlled-unitary $\texttt{ctrl-}U$ defined in equation (4.1):

$$\forall \widetilde{\mathcal{U}} \text{ unitary, } \texttt{CTRL}[\widetilde{\mathcal{U}}] = \texttt{ctrl-}U. \tag{4.22}$$

The control superchannel thus also realises, in particular, the coherent control of unitary gates.

4.4.2 Sector-preserving and controlled channels are equivalent resources

The previous section showed that there is a universal circuit structure that turns sector-preserving channels of type $(1, d)$ into their corresponding controlled channel. As resources, sector-preserving channels of type $(1, d)$ thus allow one to obtain controlled channels. We now show the opposite: from a controlled channel, one can obtain its corresponding sector-preserving channel of type $(1, d)$, once again using a universal circuit structure.

Theorem 4.4.2. *Let $\mathcal{H}_T \simeq \mathcal{H}_S^1$ be a target space, and let $\mathcal{H}_C$ be a control space of dimension 2. Taking $\mathcal{H}_S^0 \cong \mathbb{C}$, $\mathcal{H}_S^1 \simeq \mathcal{H}_T$ and $\mathcal{H}_S := \mathcal{H}_S^0 \oplus \mathcal{H}_S^1$, there exists a superchannel $\texttt{CTRL}^{-1}$ of type $(C \otimes T \to C \otimes T) \to (S \to S)$ such that for any controlled channel $\texttt{ctrl}_{C_1}\text{-}\mathcal{C}$,*

$$\texttt{CTRL}^{-1}\left[\texttt{ctrl}_{C_1}\text{-}\mathcal{C}\right] = \widetilde{\mathcal{C}}[C_1]. \tag{4.23}$$

Furthermore, this superchannel is unitary-preserving on the controlled channels on $C \otimes T$.

Proof. One can define $\texttt{CTRL}^{-1}$'s action on a given map $\mathcal{K}$ of type $C \otimes T \to C \otimes T$ as $\texttt{CTRL}^{-1}[\mathcal{K}] = \mathcal{W} \circ \mathcal{K} \circ \mathcal{V}$, where $\mathcal{V}$ is the channel corresponding to the isometry $V : \mathcal{H}_S \to \mathcal{H}_C \otimes \mathcal{H}_T$ that acts as $V |\psi\rangle = |1\rangle \otimes |\psi\rangle$ for $|\psi\rangle \in \mathcal{H}_S^1$, and $V |\psi\rangle = |0\rangle \otimes |\phi_0\rangle$ for $|\psi\rangle \in \mathcal{H}_S^0$ where $|\phi^0\rangle$ is a fixed arbitrary state in $\mathcal{H}_T$, and channel $\mathcal{W}$ acts as $\mathcal{V}^\dagger$ on $\mathcal{V}$'s range and in an arbitrary way elsewhere.

From this definition, a simple computation shows that (4.23) holds. $\qquad \square$

The existence of this inverse control superchannel shows that sector-preserving channels of type $(1, d)$ and controlled channels are fully equivalent resources: one can go from a sector-preserving channel to its corresponding controlled channel and back again, using a universal circuit architecture in both cases. This concludes our demonstration of the main claim of this chapter.

Note that $\texttt{CTRL}^{-1} \circ \texttt{CTRL}$ acts as the identity superchannel only on input channels that are sector-preserving. A way of formally restricting the $\texttt{CTRL}$ superchannel to only act on sector-preserving channels will be described in Section 4.6. Once viewed in this way, the $\texttt{CTRL}$ superchannel can be said to be unitary-preserving and invertible.

4.5 Implementing coherent control of multiple channels

4.5.1 The case of isometric channels

We now show how the previous methods apply to the coherent control of $N \geq 2$ channels, as defined in Section 4.2.2. For simplicity, we restrict ourselves to the case of isometric channels, and to $N = 2$. The methods we present are readily extendable to the $N > 2$. Note that the coherent control of isometric gates includes that of unitary gates and of pure states, as both are specific examples of isometric gates.

If we define the task of coherent control between two isometric gates as that of implementing controlled-(U, V) (as defined in (4.10)) from uses of the isometric gates U and V, then it is a direct consequence of the aforementioned no-go theorems that such a task cannot be achieved via a universal circuit architecture.

To circumvent this, we will instead keep our perspective of considering coherent control as a task performed on sector-preserving channels. Here, as in Section 4.2.2, we take the input and output target systems to be of possibly different dimensions. Accordingly, we will slightly extend the relevant definitions. For instance, Definition 4.3.1 can be extended in a straightforward way to encompass sector-preserving channels from $\mathcal{H}_{S_{\text{in}}} := \bigoplus_k \mathcal{H}^k_{S_{\text{in}}}$ to $\mathcal{H}_{S_{\text{out}}} := \bigoplus_k \mathcal{H}^k_{S_{\text{out}}}$. In the case in which the Hilbert spaces are both partitioned between a multi-dimensional sector and several one-dimensional ones, we will refer to these channels as being sector-preserving of type $(1 \to 1, \ldots, 1 \to 1, d \to d')$. Structural theorems about these channels can be seen to extend from those of Section 4.3.3 (Lemma 4.3.1, Theorem 4.3.1 and Corollaries 4.3.1 and 4.3.2) in a natural way.

In particular, Corollary 4.3.1 can be extended to a statement about isometric sector-preserving channels $\mathcal{C}$ of type $(1 \to 1, d \to d')$: they are in one-to-one correspondence with isometric operators $U_{\mathcal{C}}$ in dimension $d \to d'$. Our point is to implement this correspondence physically in order to create a control between two isometric gates. We single out a version of the control superchannel that allows one to build the coherent control between two isometric gates from the two sector-preserving isometric channels of type $(1 \to 1, d \to d')$ corresponding to these isometries. This superchannel was originally introduced in Ref. [56] (in the case $d = d'$), in a slightly different framework.

Theorem 4.5.1. *Let $\mathcal{H}_{S_{\text{in}}} = \mathcal{H}^0_{S_{\text{in}}} \oplus \mathcal{H}^1_{S_{\text{in}}}$ and $\mathcal{H}_{S_{\text{out}}} = \mathcal{H}^0_{S_{\text{out}}} \oplus \mathcal{H}^1_{S_{\text{out}}}$ be partitioned spaces, with $\mathcal{H}^0_{S_{\text{in}}}$ and $\mathcal{H}^0_{S_{\text{out}}}$ one-dimensional, let $\mathcal{H}_C$ be a control space of dimension 2, and let $\mathcal{H}_{T_{\text{in}}}$ and $\mathcal{H}_{T_{\text{out}}}$ be target spaces, with $\mathcal{H}_{T_{\text{in}}} \simeq \mathcal{H}^1_{S_{\text{in}}}$ and $\mathcal{H}_{T_{\text{out}}} \simeq \mathcal{H}^1_{S_{\text{out}}}$.*

There exists a superchannel 2-CTRL *of type* $(S_{\text{in}} \to S_{\text{out}}) \otimes (S_{\text{in}} \to S_{\text{out}}) \to (C \otimes T_{\text{in}} \to C \otimes T_{\text{out}})$ *such that for any pair of isometric sector-preserving channels $\mathcal{C}$ and $\mathcal{D}$,*

$$\text{2-CTRL}[\mathcal{C} \otimes \mathcal{D}] = \text{ctrl-}(U_{\mathcal{C}}, U_{\mathcal{D}}). \tag{4.24}$$
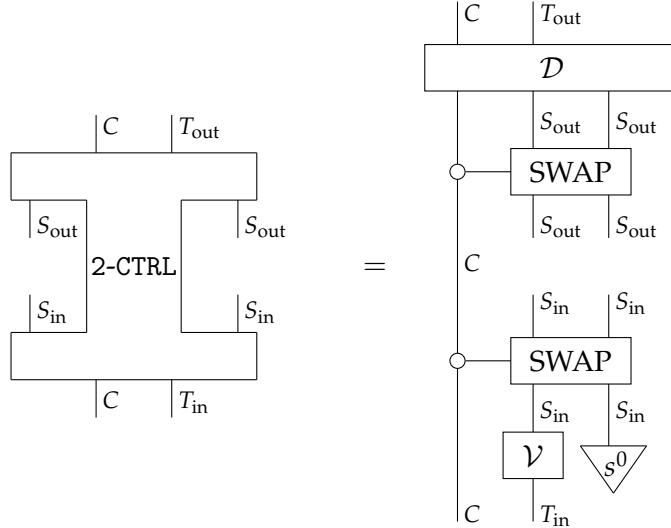
FIGURE 4.2: Quantum circuit for the 2-CTRL superchannel. The input of the superchannel are two sector-preserving channels transforming a system S_in with Hilbert space $\mathcal{H}_{S_\text{in}} = \mathcal{H}^0_{S_\text{in}} \oplus \mathcal{H}^1_{S_\text{in}}$ into a system S_out with Hilbert space $\mathcal{H}_{S_\text{out}} = \mathcal{H}^0_{S_\text{out}} \oplus \mathcal{H}^1_{S_\text{out}}$. The output of the superchannel is a controlled channel transforming the composite system $C \otimes T_\text{in}$ with $\mathcal{H}_{T_\text{in}} \simeq \mathcal{H}_{S^1_\text{in}}$ into the composite system $C \otimes T_\text{out}$ with $\mathcal{H}_{T_\text{out}} \simeq \mathcal{H}_{S^1_\text{out}}$. The channels $\mathcal{V}$ and $\mathcal{D}$ and the state $|s^0\rangle$ are defined as in Theorem 4.4.1. A very similar superchannel was defined in Ref. [56] for the case $T_\text{in} = T_\text{out}$.

Proof. This can be easily computed from the formulation of the 2-CTRL superchannel shown in Figure 4.2, in full analogy to the computation in the proof of Theorem 4.4.1. □

Theorem 4.5.1 can serve as a formalisation of the existing experimental schemes for coherently controlling two unitaries, such as the superposition of trajectories [56]. It is easy to see that it could be readily generalised to the coherent control between N isometries by a control system of dimension N.

In particular, one can see in this formulation that the coherent control of two isometries can be implemented with a simple parallel combination of the two resource sector-preserving channels.

4.5.2 What about general channels?

A natural question to ask would be whether the previous result can be extended to the case of controls between two general noisy channels, as defined in equation (4.11) and classified in Theorem 4.2.2: i.e., whether a given version of a control between two channels $\mathcal{A}$ and $\mathcal{B}$ can be obtained from the application of the 2-CTRL superchannel on suitably chosen sector-preserving channels of type $(1 \to 1, d \to d')$. The answer to this question, however, is negative.

To see this, take $\mathcal{A} = \mathcal{B} = \mathcal{D}$, where $\mathcal{D}$ is the depolarising channel on a qubit, i.e. $\mathcal{D} : \rho \mapsto \frac{1}{2}(\rho + Z\rho Z)$. One natural version of a control between $\mathcal{A}$ and $\mathcal{B}$ is then

given by the channel $\mathcal{I}_C \otimes \mathcal{D}_{S^1}$: i.e., $\mathcal{D}$ is always applied to S^1 and the control doesn't play any part. However, no use of the 2-CTRL superchannel on $\mathcal{A}$ and $\mathcal{B}$ can yield this channel. This is essentially because, in channels obtained from the use of the 2-CTRL superchannel, there can only be full coherence between one Kraus operator of $\mathcal{A}$ and one Kraus operator of $\mathcal{B}$.

Implementing the control between two noisy channels in general will therefore require the use of a more elaborate scheme, using more involved resources. In Appendix B.3, we propose such a scheme. Rather than sector-preserving channels of the form $\mathbb{C} \oplus \mathcal{H}^1_{S_{\text{in}}} \to \mathbb{C} \oplus \mathcal{H}^1_{S_{\text{out}}}$, this scheme will require the use of sector-preserving channels of the form $\mathbb{C} \oplus \mathcal{H}^1_{S_{\text{in}}} \to \mathbb{C} \oplus \mathcal{H}^1_{S_{\text{out}}} \otimes \mathcal{H}^1_E$, where $\mathcal{H}^1_E$ is an auxiliary Hilbert space, representing the environment. In such a scheme, the number of Kraus operators of $\mathcal{A}$ and $\mathcal{B}$ that can be coherent with each other in the produced controlled channel is capped by the dimension of $\mathcal{H}^1_E$.

4.6 Superchannels on routed channels

We now turn to a formal construction allowing us to describe the CTRL and 2-CTRL superchannels as acting solely on sector-preserving channels. This allows us to present in a more concise way, getting rid of irrelevant information. In particular, this yields a presentation of them as explicitly unitary protocols. We achieve this through the introduction of the notion of superchannels on routed channels.

As we saw in Section 2.4, superchannels can be conceptually defined as 'operations on operations': they are linear transformations taking quantum channels as input and mapping them to output quantum channels. Their main use is to model the different ways of using and connecting together 'black-box' operations; they provide a rigorous framework for studying the features and relative advantages of these manipulations of the black boxes.

Here, we define 'superchannels on routed channels' as superchannels which only accept a subset of all channels as input; namely, those that follow a certain route, as defined in Chapter 3 – i.e. satisfy a given set of sectorial constraints. These restrictions will make the possible superchannels more diverse, as they are no longer required to be well-defined on all possible input channels. Fortunately, a good deal of the formal work necessary in order to define such superchannels on routed channels has been undertaken already: in Ref. [17], 'deterministic supermaps' (i.e. what we call superchannels here) on a restricted subset of quantum channels were defined in general. We will recall the main parts of this definition, then apply it to the definition of superchannels on routed channels.

We denote a system X as corresponding to a finite-dimensional Hilbert space $\mathcal{H}_X$. For two systems A_{in} and A_{out}, we denote $\text{Herm}(A_{\text{in}} \to A_{\text{out}})$ to be the real vector space of Hermitian-preserving linear maps from $\mathcal{L}(\mathcal{H}_{A_{\text{in}}})$ to $\mathcal{L}(\mathcal{H}_{A_{\text{out}}})$, and $\text{QChan}(A_{\text{in}} \to A_{\text{out}})$ to be its subset containing quantum channels of type $A_{\text{in}} \to A_{\text{out}}$. We also note $\text{St}(X) \subseteq \text{Herm}(\mathcal{H}_X)$ to be the set of states for system X. The first
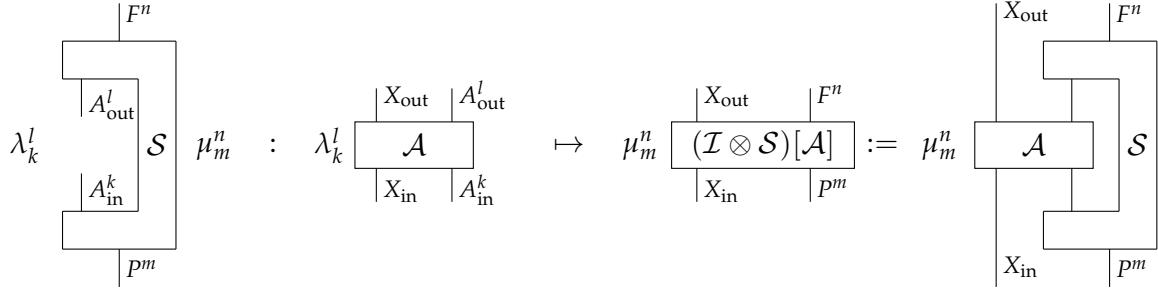
FIGURE 4.3: Diagrammatic representation of a superchannel $\mathcal{S}$ on routed channels, and of its action on a routed channel $(\lambda, \mathcal{A})$ (also acting on an auxiliary system), yielding a routed channel $(\mu, (\mathcal{I} \otimes \mathcal{S})[\mathcal{A}])$.

notion we need is that of an extension of a set of channels, which allows us to take into consideration channels which also act on an auxiliary system. Given a subset of channels $S \subseteq \mathrm{QChan}(A_{\mathrm{in}} \to A_{\mathrm{out}})$ and two systems X_{in}, X_{out}, the extension of S in $\mathrm{QChan}(A_{\mathrm{in}} X_{\mathrm{in}} \to A_{\mathrm{out}} X_{\mathrm{out}})$ is the set $\mathrm{Ext}_{X_{\mathrm{in}} \to X_{\mathrm{out}}}(S) := \{\mathcal{C} \in \mathrm{QChan}(A_{\mathrm{in}} X_{\mathrm{in}} \to A_{\mathrm{out}} X_{\mathrm{out}}) \,|\, \forall \sigma \in \mathrm{St}(X_{\mathrm{in}}), \mathrm{Tr}_{X_{\mathrm{out}}} (\mathcal{C} \circ (\mathbb{1}_{A_{\mathrm{in}}} \otimes \sigma_{X_{\mathrm{in}}})) \in S\}$. With this notion, one can define superchannels on a restricted subset of channels [17].

Definition 4.6.1 (Superchannels on a restricted subset of quantum channels)**.** *Let $S \subseteq \mathrm{QChan}(A_{\mathrm{in}} \to A_{\mathrm{out}})$ and $T \subseteq \mathrm{QChan}(P \to F)$ be subsets of channels. A superchannel of type $S \to T$ is a linear map $\mathcal{S}$ from $\mathrm{Herm}(A_{\mathrm{in}} \to A_{\mathrm{out}})$ to $\mathrm{Herm}(P \to F)$ such that, for any auxiliary systems X_{in}, X_{out} and for any channel $\mathcal{C} \in \mathrm{Ext}_{X_{\mathrm{in}} \to X_{\mathrm{out}}}(S)$, one has*

$$(\mathcal{S} \otimes \mathcal{I}_{X_{\mathrm{in}} \to X_{\mathrm{out}}})[\mathcal{C}] \in \mathrm{Ext}_{X_{\mathrm{in}} \to X_{\mathrm{out}}}(T) \,, \tag{4.25}$$

where $\mathcal{I}_{X_{\mathrm{in}} \to X_{\mathrm{out}}}$ is the identity superchannel on $\mathrm{Herm}(X_{\mathrm{in}} \to X_{\mathrm{out}})$.

We can first apply this notion to the definition of superchannels acting on a single routed channel. Here, we will restrict ourselves to routes with *full coherence*, i.e., only encoding sectorial constraints and not coherence constraints.[8]

We denote the set of channels of type $A_{\mathrm{in}} \to A_{\mathrm{out}}$ that follow the route λ as $\mathrm{QChan}^{\lambda}(A_{\mathrm{in}}^{k} \to A_{\mathrm{out}}^{l}) \subseteq \mathrm{QChan}(A_{\mathrm{in}} \to A_{\mathrm{out}})$. We will also say that these channels have type $A_{\mathrm{in}}^{k} \xrightarrow{\lambda} A_{\mathrm{out}}^{l}$; it is this type of channels on which we want to define superchannels. It is easy to prove that the condition defining the extension of $A_{\mathrm{in}}^{k} \xrightarrow{\lambda} A_{\mathrm{out}}^{l}$ to auxiliary systems can be simplified.

Lemma 4.6.1. *For a type $A_{\mathrm{in}}^{k} \xrightarrow{\lambda} A_{\mathrm{out}}^{l}$ and auxiliary systems X_{in}, X_{out}, one has:*

$$\begin{aligned} & \mathrm{Ext}_{X_{\mathrm{in}} \to X_{\mathrm{out}}}(\mathrm{QChan}^{\lambda}(A_{\mathrm{in}}^{k} \to A_{\mathrm{out}}^{l})) \\ & = \mathrm{QChan}^{\lambda}(A_{\mathrm{in}}^{k} \otimes X_{\mathrm{in}} \to A_{\mathrm{out}}^{l} \otimes X_{\mathrm{out}}) \,. \end{aligned} \tag{4.26}$$

---

[8]We will thus use the lighter notations introduced in Section 3.3.6.
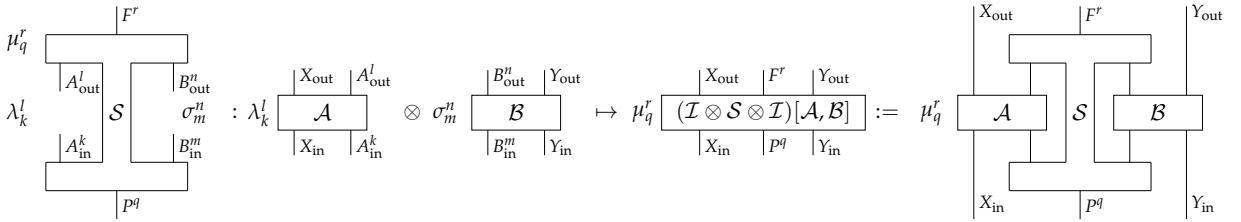
FIGURE 4.4: Diagrammatic representation of a superchannel $\mathcal{S}$ acting on a pair of routed channels $(\lambda, \mathcal{A})$ and $(\sigma, \mathcal{B})$ (also acting on auxiliary systems), yielding a routed channel $(\mu, (\mathcal{I} \otimes \mathcal{S} \otimes \mathcal{I})[\mathcal{A}, \mathcal{B}])$.

In other terms, the extension of the set of channels $A_{\text{in}} \to A_{\text{out}}$ following a route λ to a type $X_{\text{in}} \to X_{\text{out}}$ is simply the set of channels $A_{\text{in}} \otimes X_{\text{in}} \to A_{\text{out}} \otimes X_{\text{out}}$ following λ. The definition of superchannels on routed channels then derives naturally from Definition 4.6.1.

Definition 4.6.2 (Superchannel on routed channels). *Let A_{in}^k, A_{out}^l, P^m and F^n be partitioned Hilbert spaces, and let $\lambda : \mathcal{Z}_{A_{\text{in}}} \to \mathcal{Z}_{A_{\text{out}}}$ and $\mu : \mathcal{Z}_P \to \mathcal{Z}_F$ be two relations. A superchannel of type $(A_{\text{in}}^k \xrightarrow{\lambda} A_{\text{out}}^l) \to (P^m \xrightarrow{\mu} F^n)$ is a linear map $\mathcal{S}$ from $\text{Herm}(A_{\text{in}} \to A_{\text{out}})$ to $\text{Herm}(P \to F)$ such that, for any auxiliary systems X_{in}, X_{out} and for any channel $\mathcal{C} \in \text{QChan}^\lambda(A_{\text{in}}^k \otimes X_{\text{in}} \to A_{\text{out}}^l \otimes X_{\text{out}})$, one has*

$$(\mathcal{S} \otimes \mathcal{I}_{X_{\text{in}} \to X_{\text{out}}})[\mathcal{C}] \in \text{QChan}^\mu(P^m \otimes X_{\text{in}} \to F^n \otimes X_{\text{out}}). \tag{4.27}$$

We show how superchannels on routed channels can be represented graphically in Figure 4.3. The CTRL superchannel described in Theorem 4.4.1 can be characterised as a superchannel on routed channels, with type $(A^k \xrightarrow{\delta} A^l) \to (C \otimes S^1 \to C \otimes S^1)$.

Let us now turn to superchannels acting on multiple routed channels. To avoid clutter, we will present the construction for superchannels acting on a pair of channels, the generalisation to $N \geq 2$ being immediate. Formally, these have to be defined as superchannels whose input channels should be product channels, with each channel in this product following a given route. For some partitioned spaces A_{in}^k, A_{out}^l, B_{in}^m and B_{out}^n, and for two relations $\lambda : \mathcal{Z}_{A_{\text{in}}} \to \mathcal{Z}_{A_{\text{out}}}$ and $\sigma : \mathcal{Z}_{B_{\text{in}}} \to \mathcal{Z}_{B_{\text{out}}}$, we thus define $\text{ProdChan}^{\lambda \times \sigma}(A_{\text{in}}^k \otimes B_{\text{in}}^m \to A_{\text{out}}^l \otimes B_{\text{out}}^n)$ to be the intersection of the set of product channels $\text{ProdChan}(A_{\text{in}} \otimes B_{\text{in}} \to A_{\text{out}} \otimes B_{\text{out}})$ with $\text{QChan}^{\lambda \times \sigma}(A_{\text{in}}^k \otimes B_{\text{in}}^m \to A_{\text{out}}^l \otimes B_{\text{out}}^n)$. One can then define superchannels acting on such a set, once again following Definition 4.6.1.

Definition 4.6.3 (Superchannels on pairs of routed channels). *Let A_{in}^k, A_{out}^l, B_{in}^m, B_{out}^n, P^q and F^r be partitioned Hilbert spaces, and let $\lambda : \mathcal{Z}_{A_{\text{in}}} \to \mathcal{Z}_{A_{\text{out}}}$, $\sigma : \mathcal{Z}_{B_{\text{in}}} \to \mathcal{Z}_{B_{\text{out}}}$ and $\mu : \mathcal{Z}_P \to \mathcal{Z}_F$ be relations. A superchannel of type $(A_{\text{in}}^k \xrightarrow{\lambda} A_{\text{out}}^l) \otimes (B_{\text{in}}^m \xrightarrow{\sigma} B_{\text{out}}^n) \to (P^q \xrightarrow{\mu} F^r)$ is a linear map $\mathcal{S}$ from $\text{Herm}(A_{\text{in}} \otimes B_{\text{in}} \to A_{\text{out}} \otimes B_{\text{out}})$ to $\text{Herm}(P \to F)$ such that, for any auxiliary systems X_{in}, X_{out}, Y_{in}, Y_{out} and for any pair of channels $\mathcal{A} \in \text{QChan}^\lambda(A_{\text{in}}^k \otimes X_{\text{in}} \to A_{\text{out}}^l \otimes X_{\text{out}})$, $\mathcal{B} \in \text{QChan}^\sigma(B_{\text{in}}^m \otimes Y_{\text{in}} \to B_{\text{out}}^n \otimes Y_{\text{out}})$, one has*
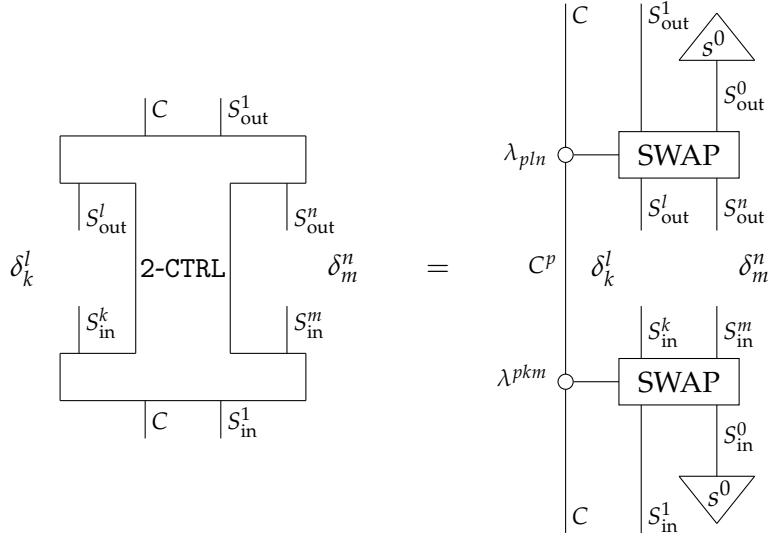
FIGURE 4.5: Fully explicit formulation of the 2-CTRL superchannel as a superchannel on sector-preserving channels, in the framework of routed quantum circuits [1]. s^0 is the only state on the one-dimensional sector $\mathcal{L}(\mathcal{H}^0_{S\text{in}})$. The Boolean vector $(\lambda^{pkm})_{p,k,m\in\{0,1\}}$ has coefficients 1 for indices 001 and 110, and 0 elsewhere. $(\lambda_{pln})_{p,l,n\in\{0,1\}}$ is its transpose. An advantage of the routed formulation is to allow one to get rid of the superfluous embedding operations that were present in the standard formulation (Figure 4.2).

$$
\begin{aligned}
&(\mathcal{I}_{X_{\text{in}}\to X_{\text{out}}} \otimes \mathcal{S} \otimes \mathcal{I}_{Y_{\text{in}}\to Y_{\text{out}}})[\mathcal{A}\otimes\mathcal{B}] \\
&\in \text{QChan}^\mu(X_{\text{in}}\otimes P^q\otimes Y_{\text{in}} \to X_{\text{out}}\otimes F^r\otimes Y_{\text{out}}).
\end{aligned}
\tag{4.28}
$$

We show how superchannels on pairs of routed channels can be represented graphically in Figure 4.4. The 2-CTRL superchannel described in Theorem 4.5.1 can be characterised as a superchannel on routed channels, with type $(A^k \xrightarrow{\delta} A^l) \otimes (A^k \xrightarrow{\delta} A^l) \to (C\otimes S^1 \to C\otimes S^1)$; we show in Figure 4.5 how it can then be written in a fully explicit way in the language of routed quantum circuits. Figure 4.5 can thus be seen as a more compact rewriting of Figure 4.2, which contained the additional operations $\mathcal{V}$ and $\mathcal{D}$. The role of these operations was simply to embed the target systems into suitable sectors. While in some specific realisations these embeddings may correspond to non-trivial physical operations, from the information-theoretic point of view they are irrelevant, and they can be completely absorbed into the graphical language of routed circuits. This is an example of how routed circuits allow for a more precise informational description of quantum protocols.

Chapter 5

Routed circuits for indefinite causal order

With their twitching, strident songs,
They strive to subdue Time

To compel it to bend its way,
To close up its curl at last...
A day shall come, the shamans say,
When Time tortuous and sly

Shall come to be entangled tight
In this laments' machinery.
And we shall be light, oh so light...
We shall have reached Eternity.

Michel Houellebecq, *The Pursuit of happiness*.

5.1   Introduction

In this chapter, we return to our main enterprise of designing frameworks to capture non-standard quantum structures, and turn to the case of indefinite causal order, which we introduced in Section 2.4.

In our view, the main challenge faced by any attempt at building a circuit framework in this context can be summarised in the following: by definition, non-ordered superchannels cannot be represented without feedback loops; but few circuits with feedback loops represent valid superchannels. One can intuitively understand this as an instance of the grandfather paradox, in which a time-traveller kills her grandfather: generically, loops in the connectivity will lead to logical inconsistencies, resulting in the non-validity of the corresponding process. Thus, what one needs is to strike a delicate middle ground: circuits featuring feedback loops, together with additional structural data from which it can be inferred that they are nonetheless consistent.

We should strive for this additional data to be minimal, and in particular, not to include the specification of the circuit's gates themselves. This is the point of a circuit framework: that it is sufficient to look at the metadata only (e.g., in standard circuits, the connectivity) to know that the architecture at hand is valid. Furthermore, we would also like this additional data, and the principles that it has to satisfy to ensure validity, to lend themselves to intuition. Finally, our framework should comprise as wide a range of scenarios as possible. A particular goalpost in this regard is the Lugano process, a paradigmatic example of a (unitary) *strongly non-causal* process, in the sense that it allows the violation of causal inequalities. As we commented on in Section 2.4.4, no other framework has been able to provide a circuit description of this process (that would guarantee its consistency) until now.

We spelled out already, in Section 2.4.3, the reasons why progress on frameworks would be highly beneficial to the field. Let us go again over the specific upshots of a circuit framework in which the consistency of processes would be readily verifiable. First, it would help us to move on from the piecemeal introduction of indefinite-order processes, to a paradigm in which one can construct large classes of processes simply by identifying the consistent circuit structures. Second, a presentation of a process in this language would immediately disclose structural facts about the core features of the process, given by the circuit's metadata, thus making its study and handling considerably less demanding. Finally, it would provide a basis for research on the general form of processes, by providing a language in which to express this general form.

Here, we show that routes are exactly what can play the role of this additional structural data. Namely, we describe a method for looking at a connectivity graph (generically including feedback loops), supplemented with the specification of sectorial constraints on the plugged-in operations, and for inferring its consistency from the satisfaction of two principles. Any circuit of this form is then valid, i.e. forms a superchannel.

The routes and connectivity, as well as the principles that they have to satisfy, are conceptually intelligible. From this framework can be derived a large class of valid unitarily extendible processes – so large that we conjecture that all unitarily extendible processes can in fact be built in this way. We provide an explicit reconstruction of the paradigmatic examples of this class: the switch, the 3-switch, the Grenoble process, and the Lugano process. The latter proves that our framework also accommodates at least some of the processes that violate causal inequalities.

We emphasise that this chapter does not aim to address the question of the *physical realisability* of processes (though its ideas might help tackle it in the future). Rather, we are interested in capturing and understanding the abstract, logical structure lying at the heart of valid processes with indefinite causal order. Building a process through our framework is not a way to certify whether it could be implemented in practice, or even in principle, given the laws of physics that govern our

particular universe. We are rather interested in whether a process is *logically conceivable* (that is, does not imply a contradiction), what makes it so, and how it can be framed in a way that makes this obvious.

The rest of the chapter is structured as follows. In Section 5.2, we begin by introducing our framework using the example of a reconstruction of the quantum switch, in order to provide a pedagogical introduction to its main notions with a simple example. In Section 5.3, we then present our circuit framework in full generality: we introduce 'routed graphs' encoding the connectivity of a circuit together with sectorial constraints, and formalise the two principle ensuring that any quantum circuit built from them defines a valid superchannel. In Section 5.4, we display how our framework allows us to reconstruct three further examples from the literature, namely the quantum 3-switch [26], the recently proposed (what we shall call) Grenoble process [84], and the Lugano process [59, 86, 87]. We embed them into larger families of similar processes, and thus highlight the conceptual intuitions for their validity. In Section 5.5, we conclude with a short discussion, in which we in particular spell out a conjecture that all unitarily extendible processes can be built using our method.

5.2 Reconstructing the quantum switch

In this section, we provide a reconstruction of the quantum switch [16, 17] that makes its consistency obvious. Of course, the switch is a simple process, whose consistency is easily demonstrated by other means; accordingly, the reconstruction we provide may be regarded as overkill in this case. The reason we discuss it is that we want to provide a pedagogical introduction to our framework's main ingredients, before we describe them more formally in Section 5.3.

In Section 2.4.2, we already introduced the switch as the paradigmatic example of a superchannel featuring indefinite causal order. In particular, Figure 2.4 presented it as a sum of two terms, each corresponding to one of the causal orders. However, if we do not want to allow for sums,[1] then it is impossible to draw $\text{SWITCH}(U, V)$ as a standard circuit in which both U and V appear exactly once, unless we allow feedback loops [16, 17, 50].

We will show how it is possible, on the other hand, to write it as an intuitive *routed* circuit. The routed circuit involves feedback loops as well, but also contains, in its routes, the necessary structural information to certify that they do not lead to logical inconsistencies. We will explain in an intuitive way how this certification can be carried out, through the study of a decorated graph – called the *routed graph* – capturing the base structure of the circuit, and checking that it satisfies two principles. Here, we gloss over technicalities, to provide the gist of the argument – a more formal treatment of our framework can be found in the next section.

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[1]This is good practice because 1) sums lead to an exponential multiplication of the number of diagrams to consider (with each of these diagrams not being a valid superchannel), and 2) an intuitive presentation as a sum will not be available at all in more involved cases, like the Grenoble process or the Lugano process.
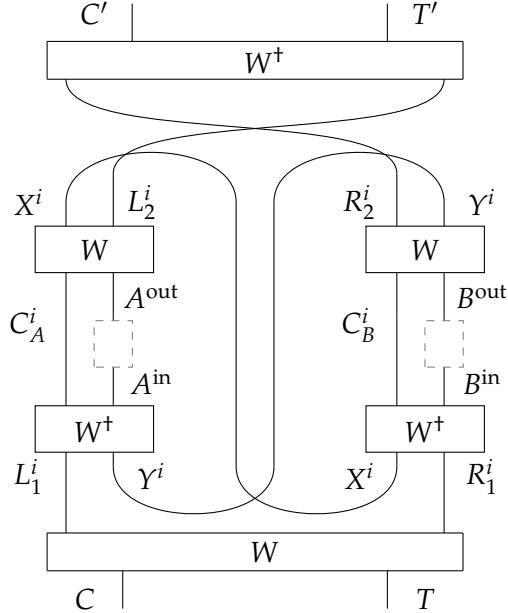
FIGURE 5.1: Routed circuit decomposition of the switch, using index matching. W is the routed unitary introduced in the main text. The wires bent into 'cup' or 'cap' shapes represent the (unnormalised) perfectly correlated entangled states (cf. Section 2.1.2). Overall, the '$i = 0$' sectors correspond to the branch where Alice's intervention is implemented before Bob's, while '$i = 1$' corresponds to the branch where Bob's intervention is implemented before Alice's. Thus the cycle is constructed from two acyclic components corresponding to definite orders of implementation.

5.2.1   Extracting the relevant structure: routed circuit decomposition, skeletal supermap, routed graph

Armed with the routed maps introduced in Chapter 3, we start by writing the switch as a routed circuit. Luckily, we only need one routed unitary for this, and it is precisely the routed map (ω, U) that we already encountered in (3.10) to model the superposition of trajectories. To achieve a more efficient presentation in the context of the present chapter, here we slightly modify our notations for it.

First, while the output sectorised spaces of (ω, U) were $\mathcal{H}_A = \mathcal{H}_A^0 \oplus \mathcal{H}_A^1$ and $\mathcal{H}_B = \mathcal{H}_B^0 \oplus \mathcal{H}_B^1$, with $\mathcal{H}_A^0 \cong \mathcal{H}_B^0 \cong \mathbb{C}$, here we will write them as $\mathcal{H}_L = \mathcal{H}_L^0 \oplus \mathcal{H}_L^1$ and $\mathcal{H}_R = \mathcal{H}_R^0 \oplus \mathcal{H}_R^1$, with $\mathcal{H}_L^1 \cong \mathcal{H}_R^0 \cong \mathbb{C}$. In other words, we swapped the labelling of the first space's sectors so that its 1-sector is now the trivial one. Accordingly, we will now write a δ route for the transformation, as opposed to the ω route used in (3.10). We will also call the map W rather than U. With index-matching, it can be represented as

$$\begin{array}{cc} L^i & R^i \\ \boxed{W} \\ C & T \end{array} \qquad . \qquad (5.1)$$
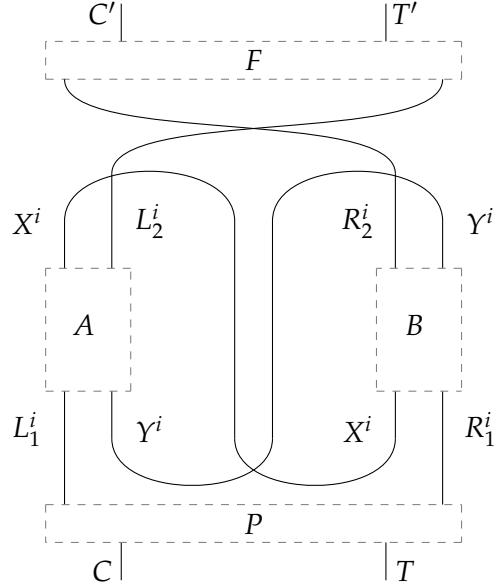
FIGURE 5.2: Skeletal supermap for the switch. The nodes suffer sectorial constraints represented by the index-matching of the input and output wires, making this a *routed* supermap. The routed circuit for the switch in Figure 5.1 is obtained by inserting the unitary transformations W and $W^\dagger$ into the nodes P and F, and the monopartite superunitary (5.2) into A and B.

Our decomposition of the switch using this map is then presented in Figure 5.1. The basic intuition behind the diagram can be informally presented in the following way. If the control qubit is prepared in $|0\rangle$, then all of the wires will have their '$i = 0$' sector instantiated. This means that some of them will reduce to describing one-dimensional dummy systems; in other words, these wires will become trivial and disappear. One can check that this leads to the circuit becoming ordered, with Alice acting before Bob. The symmetric situation arises if the control qubit is prepared in $|1\rangle$. We thus see that the route structure of this circuit precisely encapsulates the core structural features of the switch.

We now want to nail down how the route structure in Figure 5.1 can be leveraged to certify that the supermap is consistent – i.e. defines a superchannel, or here, more precisely, a superunitary. To do this, we first need to to consider a further pruned version of the circuit, in which only this essential information appears. This is given by what we call a *skeletal supermap*: a supermap that includes nothing else than wires. The idea is that we can obtain the supermap of Figure 5.1 from the skeletal supermap by 'fleshing it out', i.e. inserting some unitary transformations into the nodes. If we can show that this skeletal supermap is a superunitary, then it follows immediately that our original supermap is a superunitary.

A suitable skeletal supermap for the switch is represented in Figure 5.2. Inserting

W and $W^\dagger$ into the bottom and top nodes respectively, and inserting the superunitary
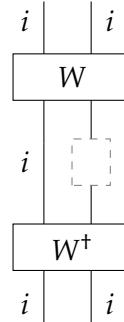
$$
\begin{array}{c}
i \quad\ \ \ i \\
\boxed{W} \\
i \quad \vdots \\
\boxed{W^\dagger} \\
i \quad\ \ i
\end{array}
\tag{5.2}
$$

into each of its two middle nodes yields the switch.

Because it encodes nothing else than sectorial constraints on its input operations, and the way in which they are connected, the skeletal supermap is in one-to-one correspondence with a decorated graph that describes this information. This is what we call the *routed graph*. It consists of

- a vertex for each node in the skeletal supermap, decorated with its route;

- arrows representing the wires connecting the nodes in the skeletal supermap;

- next to each arrow, the index of the corresponding wire;

- for each wire, the specific values of its index that correspond to a one-dimensional sector.

The routed graph for the switch's skeletal counterpart is given in Figure 5.3, with and without the index-matching shorthand. Remarkably, this elementary object contains all the information we need to confirm that the switch is a valid superunitary, or in other words, that it is consistent.

5.2.2   Checking for validity

In our framework, one can just consider the routed graph depicting the connectivity of the superchannel, and infer from it that the superchannel is valid. This amounts to checking that the routed graph conforms to a couple of principles. Here we shall present these principles and the way to check them in a pedagogical manner, taking advantage of the relative simplicity of the switch's case.

To motivate these principles, a good place to start is with the intuition that in a self-consistent protocol, information should not genuinely be able to flow in a circle. This is because, if it did, then at any point on the circle we could control the outgoing information on incoming information that is inconsistent with it. This happens in the grandfather paradox, where Alice's grandfather is killed if Alice exists, even though Alice's existence is incompatible with his murder.
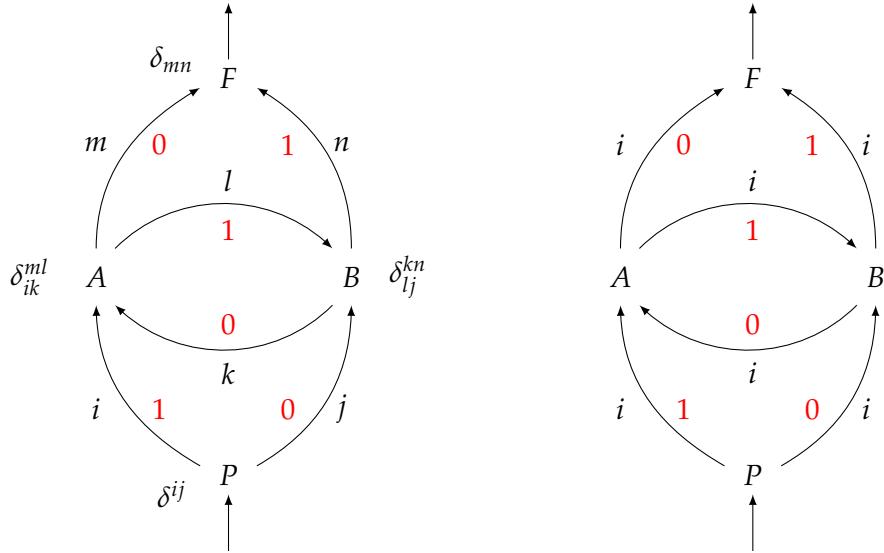
FIGURE 5.3: Routed graph for the switch, with and without index-matching. The vertices represent nodes from the skeletal supermap. On the left, each wire is equipped with its own index, and the numbers in red denote the values of the index that correspond to a one-dimensional sector. Each node is decorated with a δ matrix representing the route, which is equal to 1 if and only if all of its arguments are equal. Lower indices refer to input wires, upper indices refer to output wires. Since all the routes are 'delta' routes, we can use the convenient shorthand of index-matching to produce a simpler diagram with the same meaning, as on the right.

Yet from the present routed graph it seems as if information does flow in a circle between A and B. What we need to do is use the information in the routed graph to obtain a more fine-grained perspective from which the cycle disappears (or is at least shown to be harmless).

We start by fine-graining each node into a number of *branches*. If the route of a node dictates that there are exactly n disjoint subspaces of the input space that must be mapped one-to-one to n disjoint regions of the output space, we say that there are n branches.

To make this clear, we can look at the routes as diagrams, with arrows from the input sectors $\mathcal{H}_{\text{in}}^i$ to the output sectors $\mathcal{H}_{\text{out}}^j$ being present when the corresponding route matrix element λ_i^j is equal to 1. For the node A, we have a route of the form δ_i^j, which is represented in Figure 5.4. In this sort of diagram, each disconnected 'island', circled in red, corresponds to a distinct branch. Thus A has two distinct branches, which we label A^i in correspondence with the value of i. On the other hand, although the node P's outgoing space has two sectors, P only has one branch, since its graph is fully connected, as represented in Figure 5.5.

Intuitively, branches correspond to *alternatives* in a node: for example, in node A, either the branch A^0 or the branch A^1 will happen.[2] It is these branches, rather than

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[2]Of course, because we are in quantum theory, both could happen in a superposition. But a remarkable feature of our framework is that, in order to check the validity of the routed graph, we do
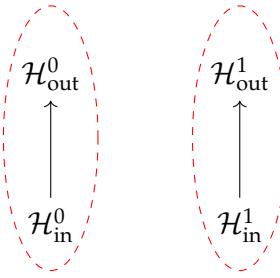
FIGURE 5.4: The route for the *A* node of the skeletal supermap.
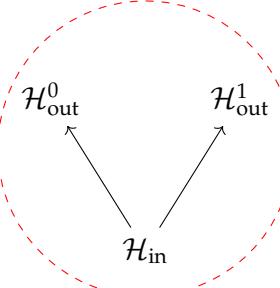
FIGURE 5.5: The route for the *P* node of the skeletal supermap.

the original nodes, that we will mainly study. In particular, we will check whether the branches themselves are in informational loops; this will be the subject of our second principle.

Bifurcation choices and Bi-univocality

But there is another thing to check before we get there. As we remarked, branches correspond to alternatives. Thus, we should make sure that the route structure is detailed enough to specify that in any given run of the process, exactly one branch happens at each node. This is captured by the notion of a *bifurcation choice*.

Let us introduce it with an example, resorting to agents for intuition. In the route for the *P* node in Figure 5.5, the ingoing space may be mapped to two different sectors of the outgoing space, meaning that an agent can 'choose' to send information to just one of these sectors. More generally, an agent at a node can make a 'bifurcation choice' for each branch of that node (for the branches that contain only one output value, the choice is trivial).

In the routed graph of Figure 5.3, only *P* features a bifurcation choice. Furthermore, this bifurcation choice amounts to picking the value of the index *i* through the graph; thus, if the agent at *P* picks, say, $i = 0$, this leads (through the other routes) to that value getting instantiated through the graph, and therefore to the branches A^0 and B^0 'happening'. The symmetric situation happens for the $i = 1$ choice. In other words, each possible bifurcation choice determines exactly one branch to happen at every node.

not have to consider superpositions: it is sufficient to reason as if the branches were mutually exclusive. Therefore this is what we will do through this section.

It is this behaviour, rather elementary in the case of the switch, that we want to ask for in general. This leads to a principle that we will call *univocality*:[3] any tuple of choices made at every branch leads to exactly one branch happening at every node. In other words, once the agents at the nodes of our skeletal supermap make all their bifurcation choices, there is a determinate fact, for each branch, about whether the quantum state will pass through it. More formally, this will be defined as the fact that the routed graph defines a function (as opposed to a relation) from bifurcation choices to 'branch statuses', where branch statuses are bits representing whether a given branch has happened or not. (Section 5.3 describes how this function is defined.) This can be seen as forbidding situations where bifurcation choices would either underdetermine branch statuses (i.e. lead to several possible branch assignments) or overdetermine them (i.e. lead to no possible assignment at all).[4]

For the switch, this is satisfied because the bifurcation choice at the *P* node of the skeletal supermap determines which branches of *A* and *B* we end up in. This corresponds to the fact that in the switch, the logical state of the control qubit fixes the causal order (recalling the fact that the causal order is what defined the different branches of *A* and *B*).

We also require that the 'time-reversed' routed graph, obtained by reversing the direction of the arrows on the original routed graph, satisfies univocality as well. This is satisfied by the switch, corresponding to the fact that the information about which causal order took place ends up recorded in the control qubit at the end of the protocol. If both the routed graph and its time-reversed version satisfy univocality, we say that the routed graph satisfies **bi-univocality**. Thus the entire bi-univocality condition is satisfied by the switch. We summarise the condition as follows:

> *Bi-univocality:* The routed graph and the time-reversed routed graph define functions from bifurcation choices to branch statuses.

The branch graph and weak loops

We now turn to our second principle, which deals with whether causal influences between branches flow in a circle. To check this, we define the *branch graph* corresponding to the routed graph; it represents the flow of information between the branches. The branch graph corresponding to the routed graph of Figure 5.3 is represented in Figure 5.6.

The branch graph features solid, dashed green, and dashed red arrows. The solid arrows represent the flow of quantum information along 'paths' in the routed graph permitted by the routes, while the dashed arrows represent the flow of information via bifurcation choices. We explain each of these in turn at an intuitive level; the

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[3]This is an unashamed gallicism. 'Univocal' means 'speaking with one voice', i.e., yielding exactly one output. For instance, functions are univocal, while relations are generically equivocal.

[4]On the relationship between underdetermination and overdetermination in cyclic processes, see Ref. [122].
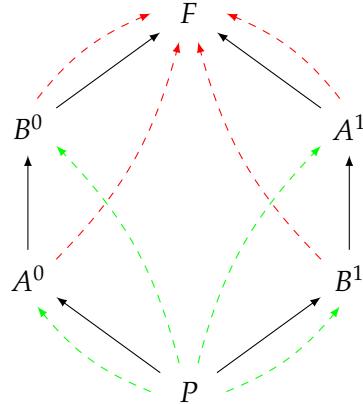
FIGURE 5.6: The branch graph for the routed graph in Figure 5.3.
Each vertex represents the branch of some node in the routed graph.
The branches of *A* and *B* are labelled with superscripts correspond-
ing to the relevant value of *i* in the index-matching routed graph. The
other nodes have only one branch, and we denote this branch with
the same letter we used for the original nodes. The solid arrows are
attributed by considering the connection between the branches en-
coded in the routed graph; the dashed green and red arrows repre-
sent relations of functional dependence in the functions from bifurca-
tion choices to branch statuses required by bi-univocality. The graph
contains no cycles of any kind, so it trivially satisfies the weak loops
condition.

general formal procedure for constructing the branch graph from a routed graph is
described in Section 5.3.

To understand the solid arrows, note that there are two possible joint value as-
signments to all of the indices in the routed graph: either $i = 0$ everywhere, or $i = 1$.
For the $i = 0$ assignment, the arrows $P \to B$ and $B \to A$ in Figure 5.3 correspond to
one-dimensional sectors, as indicated by the red zeroes. What this shows is that no
quantum information flows from P to the branch B^0 or from B^0 to A^0. For this rea-
son, there are no solid arrows $P \to B^0$ or $B^0 \to A^0$ in the branch graph. On the other
hand, quantum information does flow from P into the branch A^0, then into B^0, and
then finally into F. Thus we have the path $P \to A^0 \to B^0 \to F$ of solid arrows in the
branch graph. By following precisely analogous reasoning for the $i = 1$ assignment,
we arrive at the solid arrows in Figure 5.6. Evidently, the solid arrows in the branch
graph do not form a loop.[5]

To rule out informational loops, it is necessary that the solid arrows do not form a
loop, but it is not sufficient. What the lack of this kind of loop shows is that the quan-
tum information confined within particular branches by the routes does not flow in
a circle. But there is another type of information flowing in the routed circuit: the
information that determines *which branch happens*. This information is represented

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[5]We note that this corresponds to an observation from Ref. [75], that, although the switch has a
cyclic causal structure, it can still be written as a direct sum of (pure) processes with a definite causal
order. We want to stress however that such an observation is in general *not* sufficient to ensure the
consistency of the process, as it overlooks the need to 1) check bi-univocality, and 2) also represent
dashed arrows in the branch graph.

by the dashed arrows in Figure 5.6.

Fortunately, if univocality is satisfied, then we already know that the routed graph defines a function from bifurcation choices to the statuses of the branches (i.e. the binary variables encoding whether each branch happened). We can thus define the green dashed arrows as representing the functional dependencies within this function. Namely, there is a green dashed arrow from X^α to Y^β just in case the branch status at Y^β depends on the bifurcation choice at X^α. For example, there is a green dashed arrow from P to A^0 because one can choose whether or not A^0 happens by choosing which logical state to prepare the control qubit in at P. If a similar influence relation holds from Y^β to X^α in the time-reversed version of the protocol, then we draw a red dashed arrow from X^α to Y^β. Doing this for all the branches gives us the dashed arrows in Figure 5.6.

The full branch graph gives a complete account of the flow of information in the skeletal supermap of the switch. It represents both the quantum information that flows within the branches with the solid arrows, and the 'which-branch' information that is affected by bifurcation choices. This second sort of information can be thought of classically, since it corresponds to preferred sectorisations of the state spaces. We also call it possibilistic, since it is purely about the binary question of whether a branch does or does not happen given certain bifurcation choices, and can accordingly be represented by the routes using the theory of relations, represented by Boolean matrices.

From this fine-grained perspective, it is clear that no information actually flows in a loop in the switch, since the branch graph of Figure 5.6 satisfies

> *No loops:* There are no directed loops in the branch graph.

According to the upcoming Theorem 5.3.1 – the main theorem of this chapter –, the satisfaction of bi-univocality and no loops is enough to demonstrate the validity of the skeletal supermap of Figure 5.3, and hence of our routed circuit of Figure 5.1, representing the switch.

Remarkably though, a principle logically weaker than no loops is enough to ensure the validity of a routed circuit. We did not need to show that the routed graph contains no loops at all, but only loops of a weak, and harmless, type. Specifically, we needed to show that the graph satisfies the following principle, which we call **weak loops**.

> *Weak loops:* Any given loop in the branch graph is entirely made up of dashed arrows of a single colour.

Our main theorem states that bi-univocality and weak loops being satisfied implies that a routed graph is consistent, and hence that any routed circuit with its connectivity defines a valid superchannel. While all protocols we have studied that do not violate causal inequalities satisfy no loops, Section 5.4.3 will show that the Lugano process has green loops (see Figure 5.25). This will lead us to conjecture
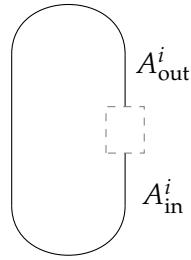
FIGURE 5.7: A routed skeletal supermap that leads to a grandfather
paradox, where a qubit is sent back to itself. Formally, the wires bent
into 'cup' and 'cap' shapes can be thought of as the unnormalised per-
fectly correlated entangled ket and bra respectively (cf. Section 2.1.1).
The qubit is partitioned into sectors spanned by the logical states $|0\rangle$
and $|1\rangle$. The index-matching means that the agent at the node must
map the logical states $|i\rangle$ to themselves, up to dephasing.

that *the presence of monochromatic loops is precisely what enables the violation of causal
inequalities*.

5.2.3   Why do we need bi-univocality?

Naively, one might imagine that the lack of a causal/informational loop among the
branches is enough to guarantee that a protocol is consistent. In this subsection, we
explain why this intuition fails.

   We start by giving an example of a skeletal supermap in which there are clearly
no causal/informational loops among the branches, and yet we still get a grand-
father paradox. The supermap is represented in Figure 5.7. In this supermap, the
two-dimensional output wire of a node is plugged into its input. The wire is parti-
tioned into sectors spanned by $|0\rangle$ and $|1\rangle$ respectively. We impose a delta-route on
the node so that the transformations we insert must map each sector to itself.

   The node has two branches, each corresponding to a one-dimensional sector.
Because of this trivial dimensionality, no information flows between the branches.
Clearly, then, there can be no question of a causal/informational loop among the
branches.

   Nevertheless, we have a grandfather paradox. Although the route prevents the
agent from generating a paradox by putting the Pauli gate $X := |1\rangle \langle 0| + |1\rangle \langle 0|$ into
the node, we can still put in $Z := |-\rangle \langle +| + |-\rangle \langle +|$ (where $|\pm\rangle := \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$).
The action of this unitary transformation on states in the $|\pm\rangle$ basis is to transform the
qubit into the opposite state to the one it was found in. This generates the paradox,
which is manifested in the fact that the supermap gives $\text{Tr}(Z) = 0$ when we insert
the Z gate into the node.

   So although we have no causal/informational loops among the branches, we
do still have a causal/informational loop, which actually leads to a paradox. The
lesson here is that the lack of causal/informational loops among branches does not
imply the lack of loops simpliciter – it may be that our choice of branch structure is

inadequate for showing that the skeletal supermap is valid. This raises the question of when a given branching structure *is* right for the job.

Our answer is: the branching structures that lead to bi-univocality being satisfied. Here, this is not the case. To see this, it is sufficient to note that there are no bifurcation choices at all, so that nothing determines which of the two branches of the node happens.

5.2.4 Summary

We offer a brief summary of this section, in which it was shown how to represent the switch in a circuit and how to certify the validity of this circuit despite its feedback loops.

We wrote the switch as a routed circuit (Figure 5.1). We captured this circuit's basic structure by trimming it down to a 'skeletal' routed supermap (Figure 5.2), from which the switch can be constructed, by inserting unitary transformations into the nodes. We represented the structure of the skeletal supermap as an equivalent routed graph (Figure 5.3). We then showed that this routed graph satisfies two conditions, bi-univocality and weak loops, which, by our main theorem, imply that the skeletal supermap is a superunitary (i.e. takes unitaries to unitaries), which in turn implies that any routed circuit with its connectivity is valid as well.

Bi-univocality requires that choices of bifurcation in the routed graph lead to a definite fact about the branch that happens at each node. It also requires a similar statement to hold about the time-reversed version of the routed graph, obtained by reversing the direction of the arrows.

If bi-univocality holds, then we can ask whether the routed graph satisfies the weak loops condition. To evaluate this condition, we form a branch graph, in which solid arrows represent the ability of quantum information to flow between the different branches. Green dashed arrows indicate that bifurcation choices at one branch can influence whether another branch happens in the routed graph. Red dashed arrows represent the same thing for a time-reversed version of the routed graph. The weak loops condition states that any given loop in the branch graph must be formed entirely of dashed arrows of the same colour. The routed graph for the switch satisfies this trivially since its branch graph contains no loops all.

5.3 The framework

In this section, we present our framework in detail and state our main theorem, which says that any routed graph satisfying bi-univocality and weak loops defines a valid superunitary. To keep things readable, we will give definitions at a semi-formal level; a fully formal account is given in Appendix C.2.

(A) An indexed graph.   (B) A routed graph.
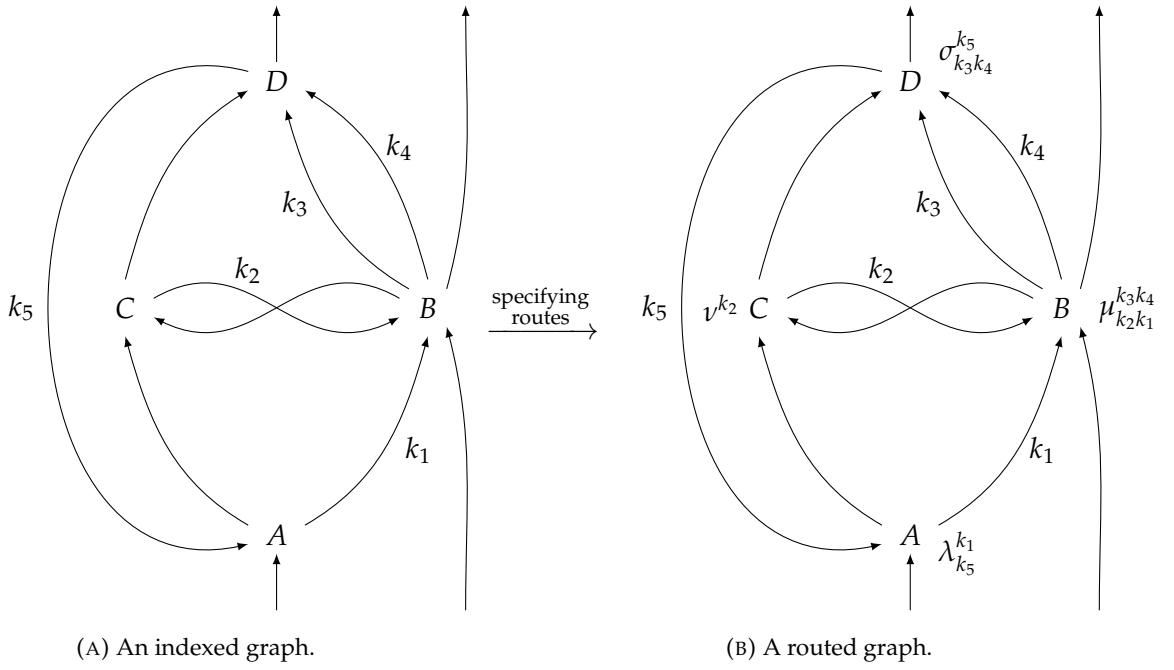
FIGURE 5.8: Examples of an indexed graph and of a routed graph;
the latter is obtained from the former by specifying a branched route
at every node. The arrows not bearing indices have a trivial (i.e. a
singleton) set of index values.

The most basic notion we need is that of a routed graph: this is a directed multi[6]-graph with decorated nodes and arrows. The nodes are decorated with routes, and the arrows are decorated with indices that are in turn equipped with a 'dimension' for each index value. A routed graph with its routes still unspecified will be called an indexed graph. Examples are given in Figure 5.8.

Definition 5.3.1 (Indexed and routed graphs)**.** *An* indexed graph Γ *is a directed multigraph in which each arrow is attributed a non-empty set of index values. Each of these values is furthermore attributed a non-zero natural number, called its dimension.*[7]

A routed graph $(\Gamma, (\lambda_N)_{N \in \mathtt{Nodes}_\Gamma})$ *is an indexed graph for which a relation (or 'route') has been specified at every node. The route λ_N at node N goes from the Cartesian product of the sets of indices of the arrows going into N, to that of the sets of indices of the arrows going out of N.*

We also allow these graphs to feature arrows 'coming from nowhere' (resp. 'going nowhere'): these will be interpreted as global inputs (resp. global outputs) of the supermap. We ask for these not to be indexed, that is, to have trivial (i.e. singleton) sets of index values.[8]

---

[6]A multigraph is a graph in which there can be several arrows between two given nodes. In the interest of generality, we will allow them, even though for the purposes of the certification of supermaps' validity, any multigraph could just be turned into an equivalent graph by merging wires.

[7]This will be the dimension of the corresponding sector in the interpretation of the graph as a supermap. Note that for our theorem, all we need to know is which sectors are one-dimensional.

[8]This requirement is there only to make the statement of univocality simpler, as otherwise one would have to distinguish several cases. Any routed graph with indexed input and output arrows can
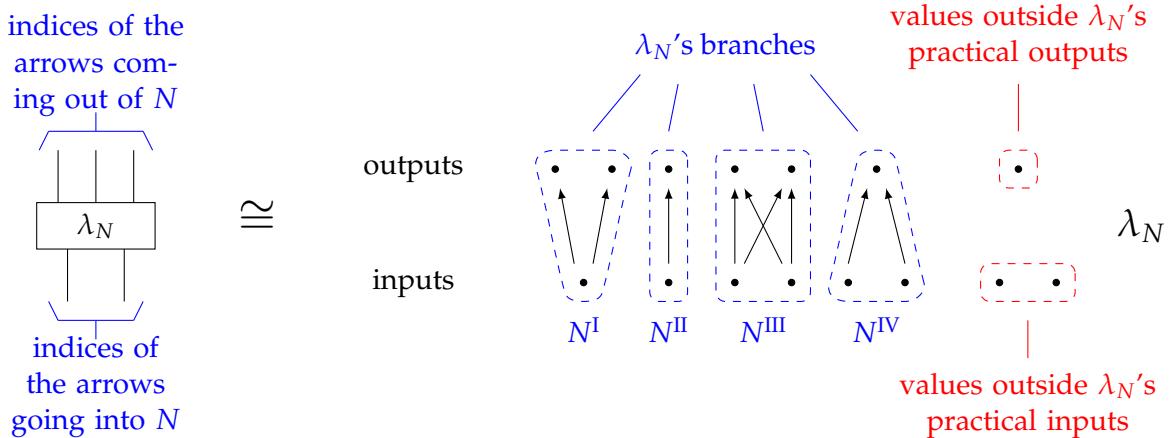
FIGURE 5.9: 'Looking inside' a branched route λ_N (which is to be used for the node N of an indexed graph). On the left, we see λ_N as a box: each of its input (resp. output) wires is the set of index values of one of the arrows going into N (resp. coming out of it). On the right, we see its 'unfolded' structure, specifying how λ_N connects input values to output values; each of the input black dots corresponds to a possible value (more precisely, a possible tuple of values) of the input indices, and similarly for the outputs.

We will in fact not need all types of relations: we will restrict ourselves to considering *branched* ones.

Definition 5.3.2 (Branched routes). *A route λ_N is* branched *if any two of its input values are either connected to the exact same output values, or have no output values in common.*

An example is given in Figure 5.9. As seen in this figure, a branched relation λ_N defines compatible (partial) partitions of its input and output sets, which we call λ_N's *branches* (or, in a slight abuse of notation, N's branches, which will be called the N^α with α varying), with each input value of a branch being connected to all output values of this branch and vice versa.

There can also be input (resp. output) values that are not connected to anything by λ_N; in line with the considerations of Section 3.1.3, these will be said to be outside its practical inputs (resp. outputs), and are considered to be part of no branch at all. These values correspond to sectors that are just there for formal purposes and will never be used in practice – part of the role of bi-univocality is to ensure that this does not lead to any inconsistency.

A skeletal routed supermap can be naturally defined from a routed graph.

Definition 5.3.3 (Skeletal supermap associated to a routed graph). *Given a routed graph $(\Gamma, (\lambda_N)_N)$, its associated skeletal (routed) supermap is obtained by interpreting each wire as a sectorised Hilbert space, whose sectors are labelled by the set of index values of this wire, with each sector having the dimension that was assigned to its corresponding index value; and interpreting each node as a slot for a linear map, going from the tensor product of*

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be turned into one without, by adjoining to it a global input node and a global output node that merge all the dangling arrows into a single, non-indexed one.
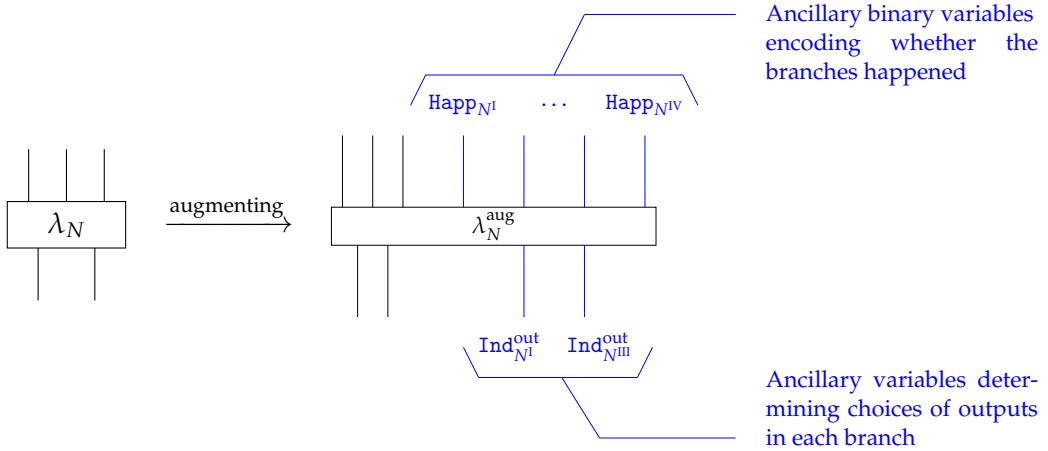
FIGURE 5.10: The 'augmented' version of the branched route λ_N described in Figure 5.9. The ancillary input wires for branches N^{II} and N^{IV} are not written, as they are trivial: each of these branches has only one output value.

the Hilbert spaces associated to its incoming arrows, to that of the Hilbert spaces associated to its outgoing arrows, and following the route associated to that node. The supermap acts on linear maps by connecting them along the graph of Γ.[9]

Our goal is to define structural requirements on routed graphs ensuring that their associated supermap is a (routed) *superunitary*; i.e., that it yields a unitary map when arbitrary unitary maps, following the routes, and possibly also acting on ancillary systems, are plugged at each of its nodes. Note that a map being unitary, in this context, means that it is unitary when restricted to act only on its practical input space, consisting of the input sectors whose indices are practical inputs of the route, and to map to its similarly defined practical output space – as discussed in Section 3.1.3.

Our first principle will be univocality. The idea is that some branches feature *bifurcations*, i.e. include several output values (e.g. branches N^{I} and N^{III} in Figure 5.9). 'Bifurcation choices', in a branch at a node – i.e. choosing a single output value for this branch, and erasing the arrows to the other output values – will in general lead to some branches at other nodes 'not happening' – i.e. to none of their input values being instantiated. Univocality tells us that *any tuple of bifurcation choices* throughout the graph should lead to *one and exactly one* branch happening at every node. To make this requirement formal, we will 'augment' our relations, i.e. supplement them with ancillary wires: ancillary input wires with which bifurcation choices in each branch can be specified; and ancillary output wires which record, in a binary variable, whether each branch happened or not.

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[9]Note that this procedure has an unambiguous meaning, despite the cycles in Γ, due to the fact that finite-dimensional complex linear maps form a traced monoidal category (and more generally, a compact closed one – see Section 2.1.2).
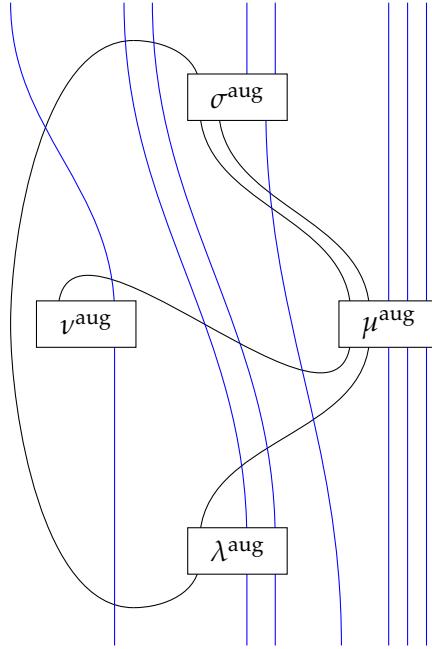
FIGURE 5.11: The 'choice relation' for the routed graph of Figure 5.8b. Here, we are assuming that ν has one branch, that λ and σ have two (with one of σ's branches having trivial bifurcation choices), and μ has three. For better readability, trivial wires are left implicit and ancillary wires are written in blue.

Definition 5.3.4 (Augmenting). *We take a branched route λ_N. For each of its branches N^α we denote the set of output values of this branch as $\mathrm{Ind}^{\mathrm{out}}_{N^\alpha}$, and define a binary set $\mathrm{Happens}_{N^\alpha} \cong \{0, 1\}$.*

The augmented *version λ^{aug}_N of λ_N is the partial function going from λ_N's input values and from the $\mathrm{Ind}^{\mathrm{out}}_{N^\alpha}$'s, to λ_N's output values and the $\mathrm{Happens}_{N^\alpha}$'s, defined in the following way:*

- *if its argument from λ_N's input values is among the input values of a branch N^α, then it returns its $\mathrm{Ind}^{\mathrm{out}}_{N^\alpha}$'s argument, value 1 in $\mathrm{Happens}_{N^\alpha}$, and value 0 in $\mathrm{Happens}_{N^{\alpha'}}$ for $\alpha' \neq \alpha$;*

- *if its argument from λ_N's input values is not among the input values of any branch – i.e. if it is outside of λ_N's practical input values –, then the output is undefined.*

As represented in Figure 5.10, the augmented version of a route features extra ancillary wires. One can then form a relation by connecting the non-ancillary wires of the λ^{aug}_N's according to the indexed graph Γ (see Figure 5.11 for an example).[10] We call this the 'choice relation', which we will write $\Lambda_{(\Gamma,(\lambda_N)_N)}$. $\Lambda_{(\Gamma,(\lambda_N)_N)}$ goes from the bifurcation choices to the $\mathrm{Happens}$ binary variables that tell us whether each branch happened. The requirement that the former unambiguously determine the latter then takes a natural form.

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[10]Similarly to before, this procedure makes sense because relations form a traced monoidal category. The λ^{aug}_N are here viewed as relations, as any partial function can be.

Principle 1 (Univocality and bi-univocality). *A routed graph* $(\Gamma, (\lambda_N)_N)$ *satisfies the principle of* univocality *if its choice relation* $\Lambda_{(\Gamma,(\lambda_N)_N)}$ *is a function.*

$(\Gamma, (\lambda_N)_N)$ *satisfies the principle of* bi-univocality *if both it and its adjoint* $(\Gamma^\top, (\lambda_N^\top)_N)$ *satisfy univocality.*

The adjoint of a routed graph is simply the routed graph obtained by reversing the direction of its arrows, and taking the adjoints of its routes: it can be interpreted as its time-reversed version. Being bi-univocal thus means being 'univocal both ways'.

When univocality is satisfied, the choice relation – which is then a choice function – plays another role: its causal structure (defined by functional dependence) tells us which bifurcation choices can affect the status of which branch. This will define the green dashed arrows in the branch graph, whereas the analogous information in the choice function of the adjoint graph will define the (reverse of the) red dashed arrows.

Our last job is to define the solid arrows in the branch graph. The idea is that the 'N^α' branch of node N has a direct influence on the 'M^β' branch of node M if there is an arrow from N to M that doesn't become either inconsistent or trivial (i.e. reduce to either zero sectors or to a single one-dimensional one) when one fixes N to be in branch α and M to be in branch β. To capture this, we will have to talk about *consistent assignments of values* to the indices of all arrows in the graph.

Definition 5.3.5 (Consistent assignment). *A consistent assignment of values to* $(\Gamma, (\lambda_N)_N)$*'s indices is an assignment of a value to the arrows' indices, such that for any node N, the tuple of values for N's inputs is related by λ_N to the tuple of values for N's outputs.*

Note that (as proven in Appendix C.2) an assignment is consistent if and only if at every node, the tuple of input values and the tuple of output values that it yields are in the same branch (and in particular are not outside the practical inputs/outputs). In that sense, one can talk about this consistent assignment of values as, in particular, assigning a given branch to every node.

The idea of solid arrows, embodied by the following definition, is then that one draws a solid arrow from N^α to M^β if there is an arrow A joining N to M, except if N^α and M^β can never happen jointly, or if there is a single value of A's index compatible with both of them happening, and this value makes A trivial.

Definition 5.3.6. *Taking a branch N^α of node N and a branch M^β of node M, we say that there is a solid arrow $N^\alpha \to M^\beta$ if there exists an arrow from N to M, except if:*

- *there are no consistent assignment of values that assign branch α to N and branch β to M;*

- *or if all such assignments assign the same value to the index of the arrow $N \to M$, and this value has dimension 1 (i.e. corresponds to a one-dimensional sector).*

If there are several arrows from N to M, then we say that there is a solid arrow $N^\alpha \to M^\beta$ unless the above applies to all of them.
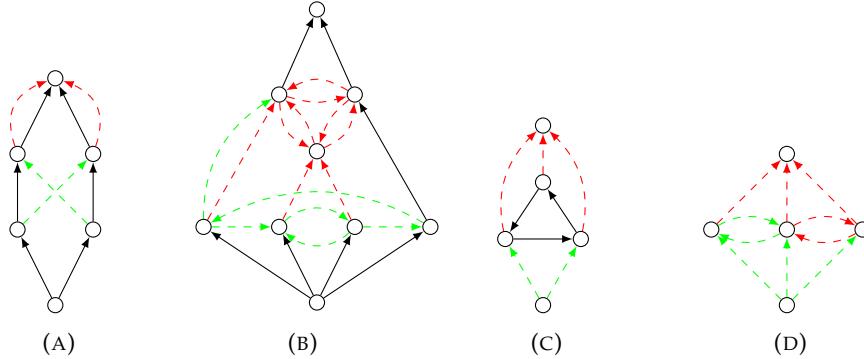
FIGURE 5.12: Examples of branch graphs. (a) and (b) satisfy the weak loops principle, but (c) and (d) do not. For (d), this is due to the presence of a bi-coloured ∞-shaped loop in the central layer.

With this in our toolbox, we can define the branch graph.

Definition 5.3.7 (Branch graph). *The* branch graph *of a routed graph* $(\Gamma, (\lambda_N)_N)$ *that satisfies bi-univocality is the graph in which:*

- *the nodes are given by the branches of* $(\Gamma, (\lambda_N)_N)$*'s nodes;*

- *solid arrows are given by the previous definition;*

- *there is a green dashed arrow* $N^\alpha \rightarrow M^\beta$ *if the choice function* $\Lambda_{(\Gamma,(\lambda_N)_N)}$ *features causal influence (i.e. functional dependence) from* $\texttt{Ind}^{\text{out}}_{N^\alpha}$ *to* $\texttt{Happens}_{M^\beta}$*;*

- *there is a red dashed arrow* $N^\alpha \rightarrow M^\beta$ *if the choice function of the adjoint graph,* $\Lambda_{(\Gamma^\top,(\lambda_N^\top)_N)}$*, features causal influence (i.e. functional dependence) from* $\texttt{Ind}^{\text{in}}_{M^\beta}$ *to* $\texttt{Happens}_{N^\alpha}$*.*

Examples of branch graphs are shown in Figure 5.12. Now that the branch graph is defined, we can check whether it satisfies our second principle.

Principle 2 (Weak loops). *We say that a loop in a branch graph is* weak *if it is entirely made of dashed arrows of the same colour.*

A routed graph satisfies the principle of weak loops if every loop in its branch graph is weak.

Note that, as a particular case, any routed graph whose branch graph features no loops trivially satisfies this principle. This will be sufficient to check the consistency of processes featuring (possibly dynamical) coherent control of causal order. We will conjecture that the more exotic processes, which violate causal inequalities, are characterised by the existence of weak loops in their branch graph.

Finally, we can display our main theorem.

Theorem 5.3.1. *Let* $(\Gamma, (\lambda_N)_N)$ *be a routed graph satisfying the principles of bi-univocality and weak loops. (We then say that it is valid.) Then its associated skeletal supermap is a routed superunitary.*

The proof of Theorem 5.3.1 is given in Appendix C.2.

The next corollary, which is direct, stresses the fact that there are then many supermaps which can be obtained from this skeletal supermap, and that the validity of the latter implies that they are valid as well.

Corollary 5.3.1. *Let* $(\Gamma, (\lambda_N)_N)$ *be a valid routed graph. Then, any supermap built from its associated skeletal supermap by plugging unitaries at some of its nodes and monopartite superunitaries at other nodes is a superunitary.*

5.4   Examples of routed circuits for processes with indefinite causal order

In this section, we reconstruct three further examples of processes with indefinite causal order as valid routed circuits, namely the quantum 3-switch, the Grenoble process and the Lugano process. This will enable us to see each of these processes as a member of a large family of processes that can be constructed 'in the same way' – i.e. that share the same basic connectivity, or in other words, are built from the same routed graph. This in turn will allow us to distinguish between those features of the process that are 'accidental', and those that are essential for the consistency of the process.

What results is reminiscent of the situation for processes without indefinite causal order. Such processes can be represented as circuits, in which it is immediate that changing the particular transformations will preserve the consistency of the process, so long as the connectivity of the circuit is maintained. The same happens in our reconstructions of processes with indefinite causal order.

In this Section, in the interest of compactness of the graphical presentation, we will make extensive use of the diagrammatic shorthand of global index constraints, presented in Section 3.2.4, from which one can infer each node's route.

5.4.1   The quantum 3-switch

The quantum 3-switch [26] is a unitary process defined analogously to the quantum switch, but with three intermediate agents: Alice (A), Bob (B) and Charlie (C). The Past (P) consists of a 6-dimensional control qudit P_C and a d-dimensional target qudit P_T. Depending on the initial state of the control qudit, the three agents receive the target qudit in a different order, outlined in Table 5.1. At the end, the target qudit is sent to the Future (F).

The routed graph

We start by drawing a routed graph from which the quantum 3-switch, amongst other processes, can be constructed. This routed graph is given in Figure 5.13. The global index constraint is represented by matching the indices on different arrows,

Control state	Order
$|1\rangle$	$A - B - C$
$|2\rangle$	$A - C - B$
$|3\rangle$	$B - C - A$
$|4\rangle$	$B - A - C$
$|5\rangle$	$C - A - B$
$|6\rangle$	$C - B - A$

TABLE 5.1: The relative order of the agents Alice (A), Bob (B) and Charlie (C) depending on the value of the control state.

and by the floating equation $l + m + n + p + q + r = 1$. This equation enforces that precisely one of the six summed-over indices is equal to one. Thus the global index constraint is the Boolean matrix that ensures that matched indices take the same value, and that exactly one of the six distinct values is 1.
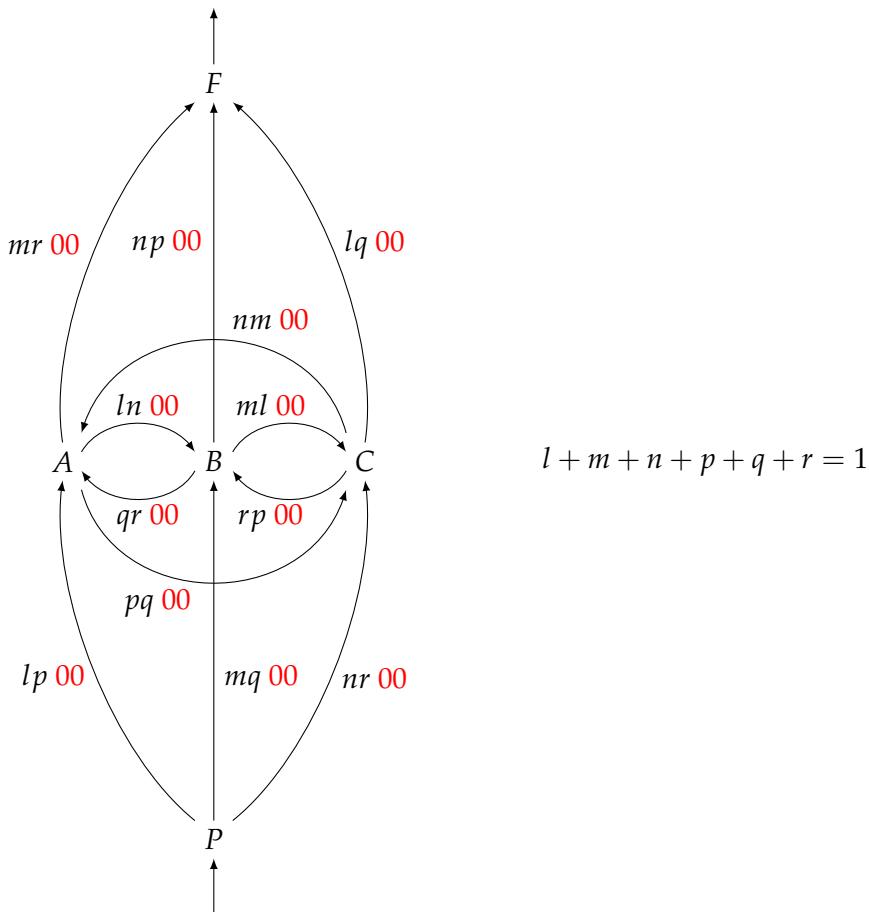
FIGURE 5.13: The routed graph for the quantum 3-switch, using a global index constraint.

The route at node P (which we denote η) is, by definition, the most liberal route compatible with the global index constraint. This is the route that forces exactly one

'A-B-C'   'A-C-B'   'B-C-A'   'B-A-C'   'C-A-B'   'C-B-A'

$\begin{cases} l = 1 \\ \text{others} = 0 \end{cases}$ $\begin{cases} p = 1 \\ \text{others} = 0 \end{cases}$ $\begin{cases} m = 1 \\ \text{others} = 0 \end{cases}$ $\begin{cases} q = 1 \\ \text{others} = 0 \end{cases}$ $\begin{cases} n = 1 \\ \text{others} = 0 \end{cases}$ $\begin{cases} r = 1 \\ \text{others} = 0 \end{cases}$

outputs   + values outside
                                                                                                                      the practical outputs

input
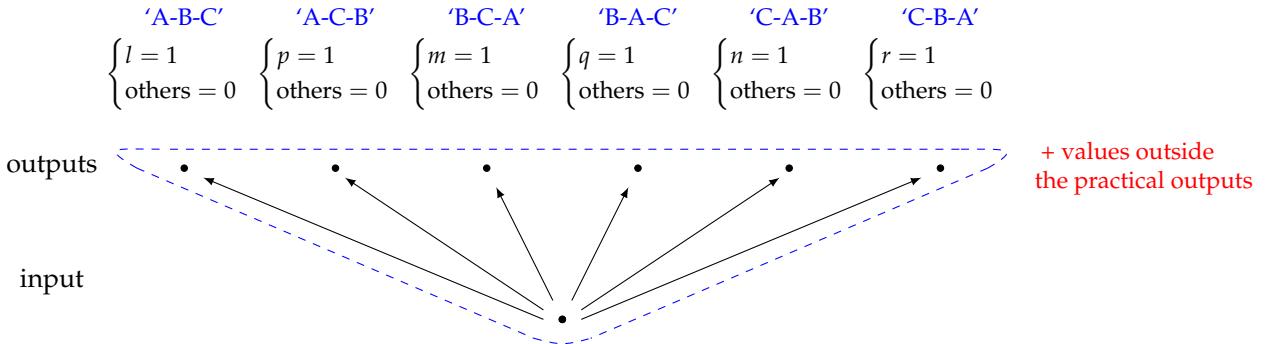
FIGURE 5.14: The route and branch structure of the node P of the quantum 3-switch. There is one unique branch with a bifurcation choice between six options, each of which enforces a causal order.

of its indices to be equal to 1:

$$\begin{cases} \eta^{100000} = \eta^{010000} = \eta^{001000} = \eta^{000100} = \eta^{000010} = \eta^{000001} = 1 \, ; \\ \eta^{lmnpqr} = 0 \quad \text{otherwise.} \end{cases} \tag{5.3}$$

The route η also has a convenient graphical representation, depicted in Figure 5.14. η has a single branch with a bifurcation choice between six options, each corresponding to one of the indices $lmnpqr$ being equal to 1. Each option enforces one of the six possible causal orders.

Let us explain how this works in detail. In the routed graph for the standard switch, the arrow $P \rightarrow A$ came with two index values, corresponding to whether or not Alice received the message first. But for the 3-switch, if Alice does receive the message first, then there are two further possibilities: either she comes first and the causal order is clockwise ($A - B - C$), or she comes first and the order is anti-clockwise ($A - C - B$). For this reason, the arrow from P to A has three index values overall. The sectors where she gets the message first correspond to ($l = 1, p = 0$) and ($l = 0, p = 1$); while ($l = 0, p = 0$) corresponds to a one-dimensional 'dummy' sector. Likewise, all internal wires are associated with three sectors; two non-'dummy' sectors for when one of their indices equals one, and a 'dummy' sector for when both are equal to zero.[11]

Now suppose that the agent at P makes the '$l = 1$' bifurcation choice, so that the message is sent to Alice. The global index constraint then enforces the route at the nodes A, B, C depicted in Figure 5.15. Thus Alice's route implies that she has no choice but to preserve the value of l, meaning that she must send the message along the arrow from A to B, since this is her only outgoing arrow that does not correspond to a dummy sector when $l = 1$. Then Bob similarly has no choice but to pass the message to Charlie, and finally Charlie is forced to send the message

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[11]Note that the sectors with both indices equal to 1, although formally present, are irrelevant: they correspond to impossible joint assignments of values.

$$\begin{cases} l = 1 \\ \text{others} = 0 \end{cases} \begin{cases} p = 1 \\ \text{others} = 0 \end{cases} \begin{cases} m = 1 \\ \text{others} = 0 \end{cases} \begin{cases} q = 1 \\ \text{others} = 0 \end{cases} \begin{cases} n = 1 \\ \text{others} = 0 \end{cases} \begin{cases} r = 1 \\ \text{others} = 0 \end{cases}$$

outputs

+ values outside the practical outputs

input

+ values outside the practical inputs

$$\begin{cases} l = 1 \\ \text{others} = 0 \end{cases} \begin{cases} p = 1 \\ \text{others} = 0 \end{cases} \begin{cases} m = 1 \\ \text{others} = 0 \end{cases} \begin{cases} q = 1 \\ \text{others} = 0 \end{cases} \begin{cases} n = 1 \\ \text{others} = 0 \end{cases} \begin{cases} r = 1 \\ \text{others} = 0 \end{cases}$$

'A-B-C'   'A-C-B'   'B-C-A'   'B-A-C'   'C-A-B'   'C-B-A'

FIGURE 5.15: The route and branch structure for the intermediate agents in the 3-switch. There are six branches, each corresponding to a causal order.

into the Future. The net result is that the message moves inexorably along the path $P \to A \to B \to C \to F$ of arrows decorated with an l index, giving the causal order $A - B - C$. Thus, if an agent at P makes the bifurcation choice that $l = 1$, they pick out this causal order.

Similarly, any option from the bifurcation choice enforces one of the six possible causal orders. In this sense, the bifurcation choice at P is a choice between causal orders, just as in the case of the original quantum switch. This state of affairs – that the causal order is determined by a bifurcation choice at the Past node – is characteristic of the (non-dynamical) coherent control of causal orders.

Now let us show that the routed graph satisfies our two principles. It is clear that the bifurcation choice at P, picking which index is equal to 1, determines the status of all branches of the intermediate nodes, since these branches are all defined by a certain index equalling 1 (see Figure 5.15). This bifurcation choice is the only one in the routed graph, and P and F each have just one branch (the route at F is just the time-reversed version of the one at P, obtained by reversing the direction of the arrows in Figure 5.14). Thus the sole bifurcation choice in the routed graph leads to a single branch happening at each node; formally speaking, we have a function from bifurcation choices to branch statuses. That is, the routed graph satisfies univocality. Since the routed graph is time-symmetric, it follows that it satisfies bi-univocality. This allows us to draw the branch graph, following the rules in Section 5.2.2: we display it in Figure 5.16. In this graph, the six branches for each of the nodes A,B and C are denoted by the specification of which index is equal to 1 (with all the others equal to 0), e.g. $A^{l=1}$, $A^{p=1}$, etc. There are no loops in the branch graph, meaning that the routed graph trivially satisfies weak loops. We can thus invoke Theorem 5.3.1 to conclude that any process that can be obtained from the routed graph of Figure 5.13, including the quantum 3-switch, is a consistent quantum process.
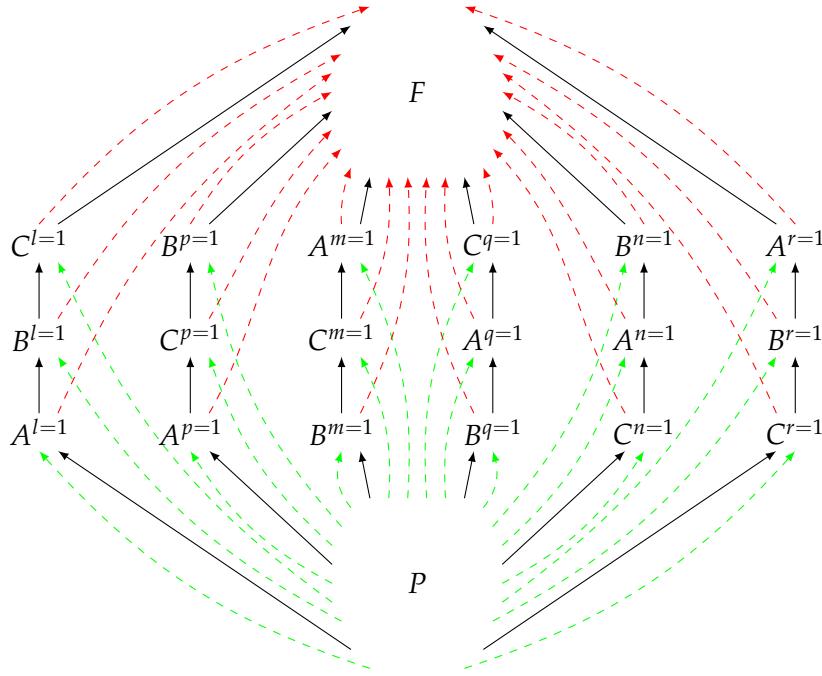
FIGURE 5.16: The branch graph for the quantum 3-switch.

The routed circuit

The routed circuit for the quantum 3-switch can be constructed from the routed graph in Figure 5.13 by inserting unitary transformations into the corresponding skeletal supermap. This is displayed in Figure 5.17, where we have again used the shorthand of global index constraints. The routes of the transformations can be derived from the global index constraint, just like the routes of the nodes in the routed graph.

The systems in the routed circuit have the following properties:

- The systems $P_T, F_T, A_{\text{in}}, A_{\text{out}}, B_{\text{in}}, B_{\text{out}}, C_{\text{in}}, C_{\text{out}}$ are all isomorphic, and correspond to a d-dimensional space.

- P_C, F_C are 6-dimensional control systems.

- The routed system C_k is also a 6-dimensional control system, with an explicit partition into six one-dimensional sectors.

- The routed systems $R^{lp}, S^{mq}, T^{nr}, X^{ln}, Y^{pq}$ are all $(2d+1)$-dimensional systems, this time partitioned into *two d-dimensional sectors* and a single 1-dimensional 'dummy' sector. For example, $R^{lp} = R^{00} \oplus R^{10} \oplus R^{01}$, where R^{00} is the 1-dimensional sector. The presence of two separate d-dimensional sectors corresponds to the fact that each of these wires can carry the message in two separate causal orders. We denote the unique state in the 1-dimensional sectors by $|\text{dum}\rangle$.
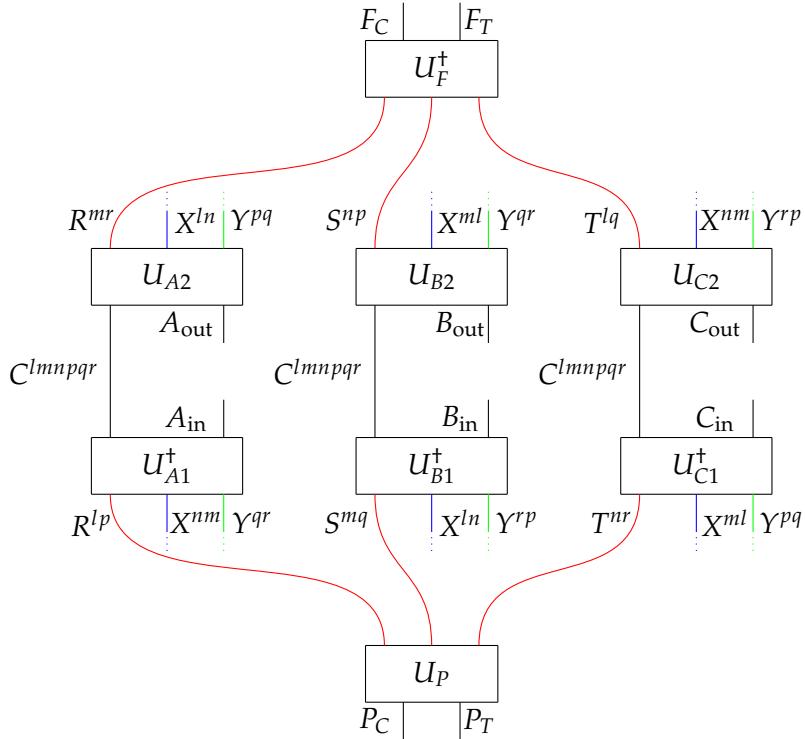
$$l + m + n + p + q + r = 1$$

FIGURE 5.17: A routed circuit diagram for the quantum 3-switch, using a global index constraint. To avoid too much clutter, instead of explicitly drawing loops, output lines that end with dots are to be interpreted as being looped back to join the corresponding input lines with dots (with the same system labels, including indices). Some wires are coloured for readability.

The unitary U_P at the bottom of the diagram is given by the isomorphism:

$$
U_P :
\begin{cases}
|1\rangle_{P_C} \otimes |\psi\rangle_{P_T} \mapsto |\psi\rangle_{R^{10}} \otimes |\text{dum}\rangle_{S^{00}} \otimes |\text{dum}\rangle_{T^{00}} \\[4pt]
|2\rangle_{P_C} \otimes |\psi\rangle_{P_T} \mapsto |\psi\rangle_{R^{01}} \otimes |\text{dum}\rangle_{S^{00}} \otimes |\text{dum}\rangle_{T^{00}} \\[4pt]
|3\rangle_{P_C} \otimes |\psi\rangle_{P_T} \mapsto |\text{dum}\rangle_{R^{00}} \otimes |\psi\rangle_{S^{10}} \otimes |\text{dum}\rangle_{T^{00}} \\[4pt]
|4\rangle_{P_C} \otimes |\psi\rangle_{P_T} \mapsto |\text{dum}\rangle_{R^{00}} \otimes |\psi\rangle_{S^{01}} \otimes |\text{dum}\rangle_{T^{00}} \\[4pt]
|5\rangle_{P_C} \otimes |\psi\rangle_{P_T} \mapsto |\text{dum}\rangle_{R^{00}} \otimes |\text{dum}\rangle_{S^{00}} \otimes |\psi\rangle_{T^{10}} \\[4pt]
|6\rangle_{P_C} \otimes |\psi\rangle_{P_T} \mapsto |\text{dum}\rangle_{R^{00}} \otimes |\text{dum}\rangle_{S^{00}} \otimes |\psi\rangle_{T^{01}}
\end{cases}
\tag{5.4}
$$

between the non-routed system $P_C \otimes P_T$ (6d-dimensional) and the routed system $\bigoplus_{lmnpqr} \eta^{lmnpqr} R^{lp} \otimes S^{mq} \otimes T^{nr}$ [also of dimension $2(d \times 1 \times 1) + 2(1 \times d \times 1) + 2(1 \times 1 \times d) = 6d$].

U_F has the same form as U_P, where the $|1\rangle_{F_C}$ state of the control qubit is again mapped to the $l = 1$ sector, $|2\rangle_{F_C}$ is again mapped to $p = 1$ sector, and so on. The other unitaries denoted by U are the unique unitaries of the form above that respect the index-matching.

5.4.2   The Grenoble process

In their 2021 paper [84], Wechs and co-authors from Grenoble presented a new tripartite process with *dynamical* indefinite causal order, that is, where the causal order is not predetermined at the start of the process, but can be influenced by the intermediate agents themselves. In the present work, we shall call this process the *Grenoble process*.

Like the 3-switch, the Grenoble process involves three intermediate agents, who receive information from the global Past and ultimately send information into the global Future.[12] The Past (P) consists of a 3-dimensional control qutrit P_C and a 2-dimensional target qubit P_T. As with the previous processes we have studied, the logical state of the control system determines which of the intermediate agents will receive the message first. However, unlike the previous processes, this control system does not enforce a single causal order. This is because the agent who receives the message first is free to choose which agent will receive it second. In particular, the logical state of the target qubit after it passes through the first node will determine who gets it second: $|0\rangle$ means it will be sent in clockwise order (for example, to Bob if Alice was first), while $|1\rangle$ means it will be sent in anticlockwise order (for example, to Charlie if Alice was first). Finally, before the action of the third and final agent, the information about the relative order of the first two agents is scrambled onto an ancillary qubit, which is transferred directly to the Future (F).

In the Grenoble process, the emergent causal order depends not only on the global Past, but also on the actions of the intermediate agents. This is the hallmark of *dynamical* coherent control of causal order. In our terms, this will correspond to the fact that a causal order (and the branch statuses that fix it) is determined not only by a bifuraction choice at the Past, but also by bifurcation choices of the intermediate agents.

The routed graph

To begin with, we write down a routed graph from which the Grenoble process, amongst others, can be constructed. This graph is given in Figure 5.18, again using a global index constraint.

For each arrow, the sector corresponding to all of its indices being equal to zero is a one-dimensional sector. The global index constraint (in particular, the floating equation $l + m + n = 1$), imposes a route at the node P that forces exactly one of the outgoing indices to equal 1, depicted in Figure 5.19. The route at the F node is just the time-reverse of the route at the Past. The global index constraint also gives rise to a route at A depicted in Figure 5.20. The routes at B and C are closely analogous.

Just like the routed graph for the 3-switch, the bifurcation choice at P determines which agent comes first. But unlike the 3-switch, this bifurcation does not enforce

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[12]Note, that in the original formulation in Ref. [84], the Future is split into more than one party, whilst in this work, to simplify the presentation we consider only one Future party.
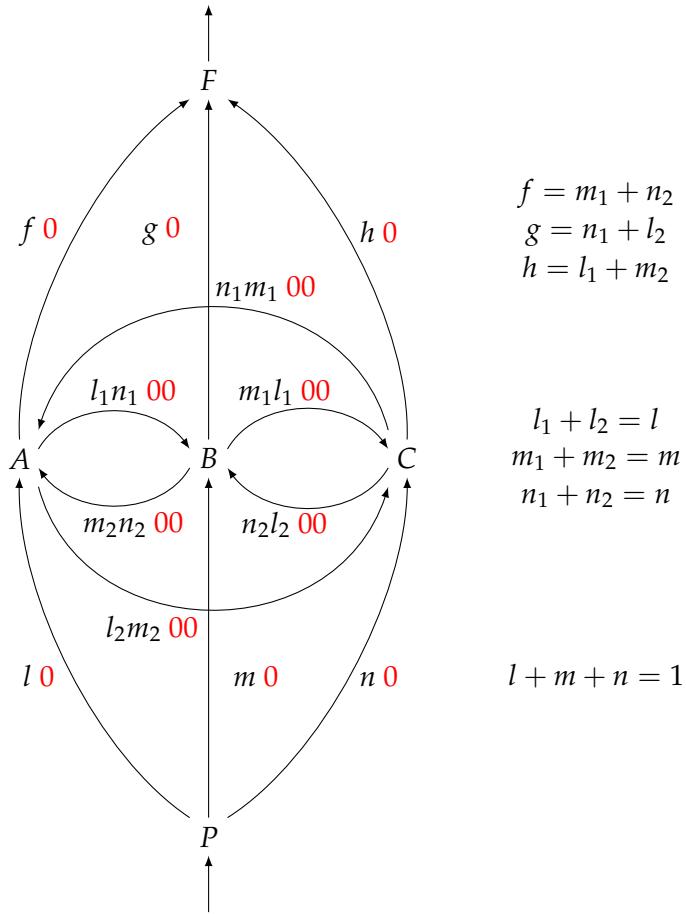
FIGURE 5.18: The routed graph for the Grenoble process, using a global index constraint.

an entire causal order. Rather, it is left to the first intermediate agent to decide which one should come second. For example, suppose that an agent at P makes the bifurcation choice $l = 1$. This sends the message to Alice (since the only outgoing arrow from P that is not associated with a trivial dummy sector in this case is $P \rightarrow A$). This leads to Alice having the binary bifurcation choice associated with the branch $A^{l=1}$, depicted in Figure 5.20. This bifurcation choice determines which agent comes second. For example, suppose Alice chooses the bifurcation option $l_1 = 1$. Then the message is passed along the '$l_1 n_2$'-indexed arrow to Bob. Then Bob's route implies he has no such choice: he is forced to preserve the value of $l_1 = 1$, and is thereby compelled to send the message along the $m_1 l_1$ arrow to Charlie (he is confined to a branch $B^{l_1=1}$, analogous to $A^{n_1=1}$ in Figure 5.20). Finally, Charlie, confined to a branch $C^{h=1}$ analogous to $A^{f=1}$ in Figure 1, is forced to send the message off into the Future. Thus Alice's choice $l_1 = 1$ enforces the clockwise causal order $A - B - C$. On the other hand, choosing $l_2 = 1$ leads to the anticlockwise order $A - C - B$.

The situation is analogous if another one of the agents comes first. If Bob comes first, he makes a bifurcation choice between $m_1 = 1$ and $m_2 = 1$ that enforces either the clockwise order $B - C - A$ or the anticlockiwse order $B - A - C$, respectively. Finally, if Charlie comes first, he chooses between $n_1 = 1$ and the clockwise order

'Alice comes   'Bob comes   'Charlie comes
   first'   first'   first'

$$\begin{cases} l = 1 \\ \text{others} = 0 \end{cases} \qquad \begin{cases} m = 1 \\ \text{others} = 0 \end{cases} \qquad \begin{cases} n = 1 \\ \text{others} = 0 \end{cases}$$

outputs   + values outside
                                                            the practical outputs

input
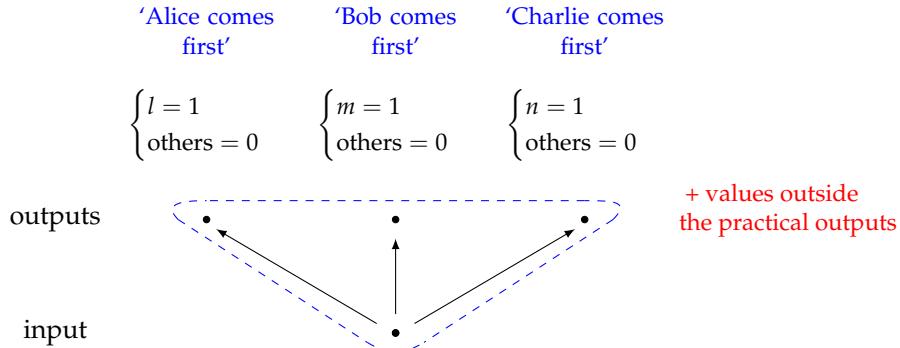
FIGURE 5.19: The branch structure for the node P of the Grenoble process. The bifurcation choice in the unique branch determines which agent comes first.

$$\begin{cases} l_1 = 1 \\ \text{others} = 0 \end{cases} \quad \begin{cases} l_2 = 1 \\ \text{others} = 0 \end{cases} \quad \begin{cases} n_1 = 1 \\ \text{others} = 0 \end{cases} \quad \begin{cases} m_2 = 1 \\ \text{others} = 0 \end{cases} \quad \begin{cases} f = 1 \\ \text{others} = 0 \end{cases}$$

outputs   + values outside
                                                                              the practical outputs

inputs   + values outside
                                                                              the practical inputs

$$\begin{cases} l = 1 \\ \text{others} = 0 \end{cases} \qquad \begin{cases} n_1 = 1 \\ \text{others} = 0 \end{cases} \quad \begin{cases} m_2 = 1 \\ \text{others} = 0 \end{cases} \quad \begin{cases} m_1 = 1 \\ \text{others} = 0 \end{cases} \quad \begin{cases} n_2 = 1 \\ \text{others} = 0 \end{cases}$$

$A^{l=1}$
'Alice comes first, chooses who comes second'

$A^{n_1=1}$
'Alice comes second, after Charlie'

$A^{m_2=1}$
'Alice comes second, after Bob'

$A^{f=1}$
'Alice comes last'

FIGURE 5.20: The branch structure for the node A of the Grenoble process.

order $C - A - B$, or $n_2 = 1$ and the anticlockwise order $C - B - A$.

This scenario also allows for the disappearance of the information about the order of agents that acted already. Indeed, suppose that Alice comes last. This means she has either received the message coming clockwise from Charlie, or anticlockwise from Bob: i.e., either $m_1 = 1$ or $n_2 = 1$, respectively. In both cases, the floating equation $f = m_1 + n_2$ guarantees that $f = 1$, meaning that the information about which agent came first and which came second is lost.[13] This can be seen in the structure of the '$f = 1$' branch in Figure 5.20. Again, the situation is analogous if another agent comes last.

To construct the branch graph, consider the following. The node P consists of a single branch with a bifurcation choice between three options, each corresponding to the case when one of the three indices l, m, n equals 1. In the time-reversed version of the routed graph, the node F has a bifurcation with three options, each corresponding to the case when one of the three indices f, g, h equals 1.

The routes at the nodes A, B, C consist of four branches, as illustrated in Figure 5.20. One of these branches corresponds to the case when the index on the wire coming directly from P equals 1, with a bifurcation between two options splitting this index into an index of the same name with subscript either 1 or 2 (corresponding to whether the message is sent clockwise or anticlockwise). Another branch corresponds to the case when the index on the wire going directly to F equals 1, with a bifurcation in the time-reversed routed graph combining the second index of each of the two wires coming in from the other agents (corresponding to whether the message came from the clockwise or anticlockwise direction). The final two branches correspond to the cases when one of the two indices that appear on both the input and output wires of the nodes are equal to 1. Following Figure 5.20, we shall denote these branches by superscripts labelling which index is equal to 1.

The fact that the routed graph satisfies univocality is implicit in the above explanation of how the bifurcation choices pick out a causal order. For they do so precisely by determining which branch happens at each node. For example, the bifurcation choice $l = 1$ at P leads to the branch $A^{l=1}$ happening, corresponding to Alice coming first. Then Alice's bifurcation choice determines which branches happen at B and C: $B^{l_1=1}$ and $C^{h=1}$ if she chooses $l_1 = 1$; $C^{l_2=1}$ and $B^{g=1}$ if she chooses $l_2 = 1$. In general, the bifurcation choices at P and at the resulting first intermediate node always determine which branches happen. Thus, the routed graph satisfies univocality. Since the routed graph is time-symmetric, it immediately follows that it satisfies bi-univocality.

This allows us to draw the branch graph, which is shown in Figure 5.21. Since this branch graph has no loops, it trivially satisfies our weak loops condition. Thus the routed graph is valid. It follows that the Grenoble process – and any other process constructed from this routed graph – is consistent.

---

[13]More specifically, this information is not tracked anymore by the route structure. Of course, depending on Alice's choice of intervention, this information could still be sent to the Future and be read there; but the scenario does not ask for it to be preserved in a specific structural way.
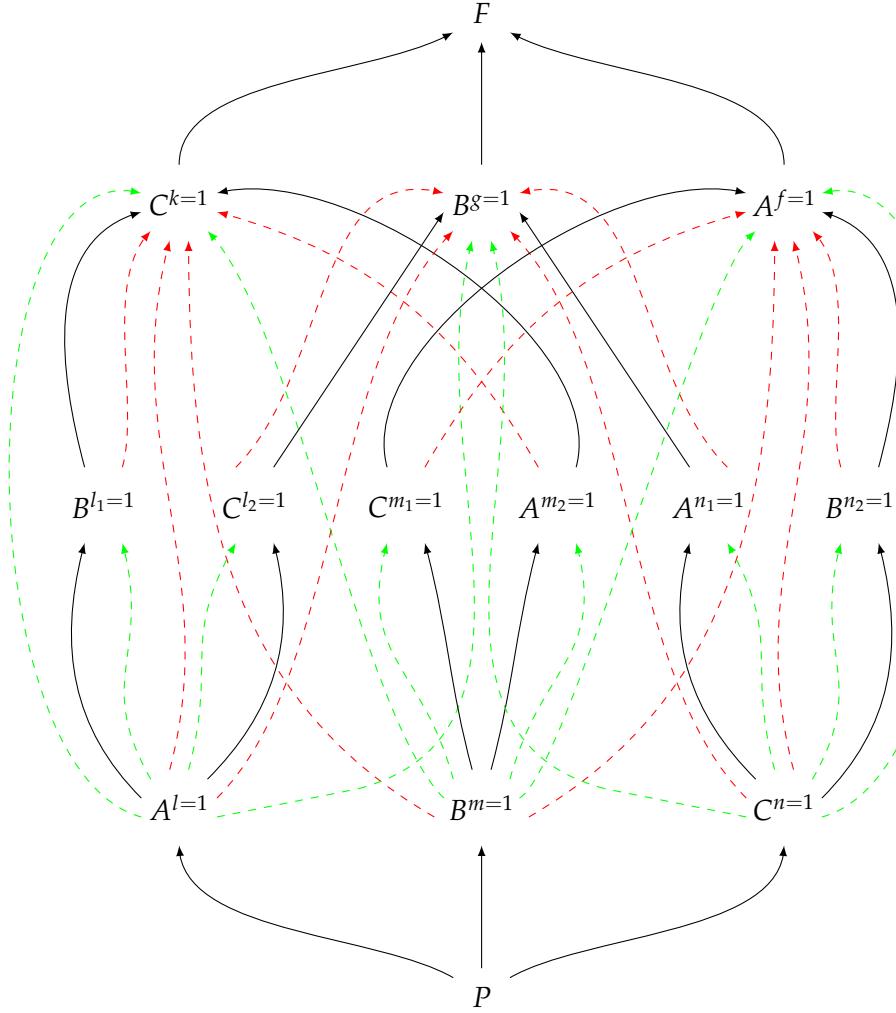
FIGURE 5.21: The branch graph for the Grenoble process. For clarity, we have omitted the green and red dashed arrows from P and to F, respectively: they simply point upwards in the diagram to/from all of the other branched nodes.

Routed circuit

By inserting suitable unitary transformations into the skeletal supermap associated with Figure 5.18, we can now construct the Grenoble process. A routed circuit for the Grenoble process is given in Figure 5.22:

- The systems $P_T, F_T, A_{\text{in}}, A_{\text{out}}, B_{\text{in}}, B_{\text{out}}, C_{\text{in}}, C_{\text{out}}$ are all isomorphic, and correspond to a 2-dimensional target Hilbert space (encoding the message).

- P_C is a 3-dimensional control system; F_C is a 3-dimensional control system, F_A is a 2-dimensional ancillary system.

- The routed systems $Q^{fln_1m_2}, Q^{gml_1n_2}, Q^{hnm_1l_2}$ are 4-dimensional control systems, with an explicit partition into four 1-dimensional sectors, each corresponding to exactly one of their four indices being equal to one.
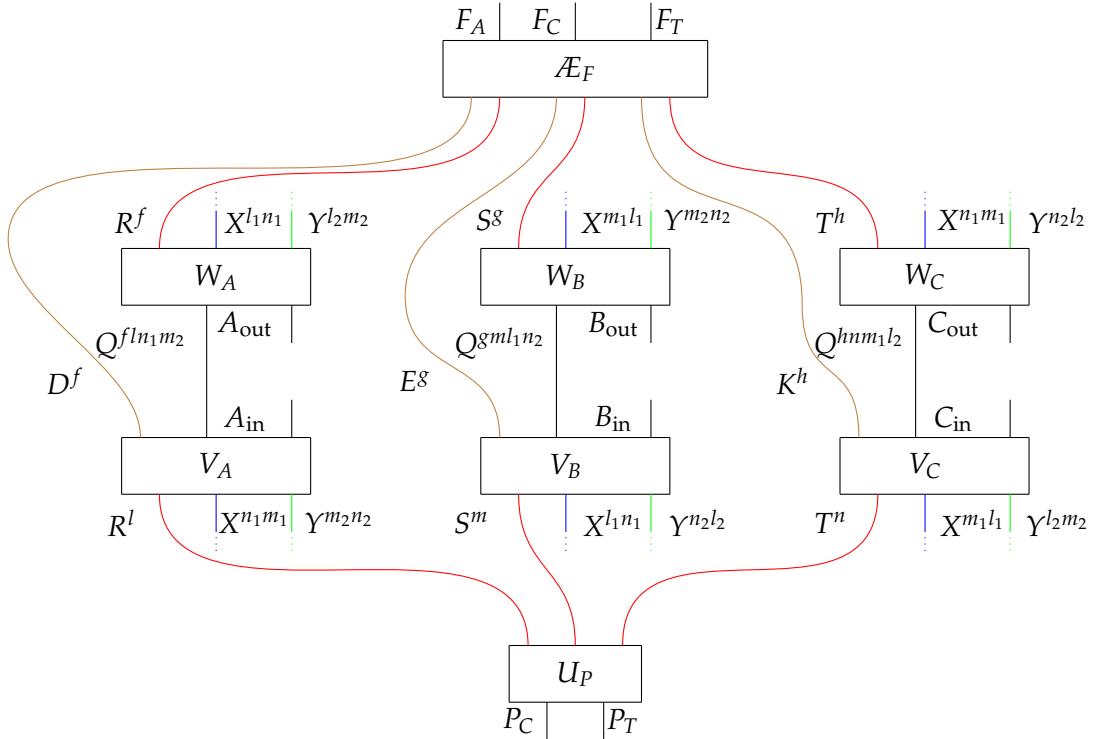
FIGURE 5.22: A routed circuit diagram for the Grenoble process, using a global index constraint. To avoid graphical clutter, we have avoided explicitly drawing loops. Instead, output lines that end with dots are to be interpreted as being looped back to join the corresponding input lines with dots (with the same system labels, including indices). Wires are coloured for better readability.

- The routed systems $R^l, R^f, S^m, S^g, T^n, T^h$ are 3-dimensional systems, with an explicit partition into one 1-dimensional 'dummy' sector and one 2-dimensional 'message' sector, for example, $R^l = R^0 \oplus R^1$, where R^0 is the 1-dimensional sector.

- The routed systems D^f, E^g, K^h are similarly 3-dimensional systems, with an explicit partition into one 1-dimensional 'dummy' sector and one 2-dimensional 'ancillary' sector, for example, $D^l = D^0 \oplus D^1$, where D^0 is the 1-dimensional sector. The 2-dimensional 'ancillary' system will be used to store the information about whether the message was sent clockwise or anticlockwise after the first agent, conditional on the state of the qubit before the action of the third agent.

- The routed systems $X^{n_1 m_1}, Y^{m_2 n_2}, X^{l_1 n_1}, Y^{n_2 l_1}, X^{m_1 l_1}, Y^{l_2 m_2}$ are all 4-dimensional systems, partitioned into *one* 2-dimensional 'message' sector (corresponding to

the message travelling from the second to the third agent), *one* 1-dimensional 'message' sector (corresponding to the message travelling from the first to the second agent, in which case the space is only one-dimensional because the state of the message itself determines to whom it is sent next), and *one* 1-dimensional 'dummy' sector. For example, $X^{n_1 m_1} = X^{00} \oplus X^{10} \oplus X^{01}$, where X^{00} is the 1-dimensional 'dummy' sector and X^{10} is the 1-dimensional 'message' sector.

The global index imposes a route $\delta^{(l+m+n),1}$ on U_P that forces exactly one of its output indices to be equal to 1. In other words, its practical output space is $\bigoplus_{lmn} \delta^{(l+m+n),1} R^l \otimes S^m \otimes T^n$.

U_P is a three-party generalisation of the superposition-of-trajectories unitary (5.1) from Section 5.2. Its action is given by the following, where we label the kets by individual sectors, rather than by systems:

$$
U_P : \begin{cases}
|1\rangle_{P_C} \otimes |\psi\rangle_{P_T} \mapsto |\psi\rangle_{R^1} \otimes |\text{dum}\rangle_{S^0} \otimes |\text{dum}\rangle_{T^0} \\
|2\rangle_{P_C} \otimes |\psi\rangle_{P_T} \mapsto |\text{dum}\rangle_{R^0} \otimes |\psi\rangle_{S^1} \otimes |\text{dum}\rangle_{T^0} \\
|3\rangle_{P_C} \otimes |\psi\rangle_{P_T} \mapsto |\text{dum}\rangle_{R^0} \otimes |\text{dum}\rangle_{S^0} \otimes |\psi\rangle_{T^1}
\end{cases}
\tag{5.5}
$$

Thus U_P defines a unitary transformation from $P_C \otimes P_T$ to $\bigoplus_{lmn} \delta^{(l+m+n),1} R^l \otimes S^m \otimes T^n$. In fact, the global index constraint (in particular, the floating equation $l + m + n = 1$) restricts U_P's practical output space to $\bigoplus_{lmn} \delta^{(l+m+n),1} R^l \otimes S^m \otimes T^n$, meaning that it defines a routed unitary transformation.

V_A is defined below. Note that here the labelling by sectors is necessary to distinguish between states belonging to different sectors that we label with the same ket, e.g. $|0\rangle_{X^{01}}$ and $|0\rangle_{X^{10}}$.

$$
V_A : \begin{cases}
|0\rangle_{R^1} \otimes |\text{dum}\rangle_{X^{00}} \otimes |\text{dum}\rangle_{Y^{00}} \mapsto |0\rangle_{A_{\text{in}}} \otimes |0\rangle_Q \otimes |\text{dum}\rangle_{D^0} \\
|1\rangle_{R^1} \otimes |\text{dum}\rangle_{X^{00}} \otimes |\text{dum}\rangle_{Y^{00}} \mapsto |1\rangle_{A_{\text{in}}} \otimes |0\rangle_Q \otimes |\text{dum}\rangle_{D^0} \\
|\text{dum}\rangle_{R^0} \otimes |0\rangle_{X^{10}} \otimes |\text{dum}\rangle_{Y^{00}} \mapsto |0\rangle_{A_{\text{in}}} \otimes |1\rangle_Q \otimes |\text{dum}\rangle_{D^0} \\
|\text{dum}\rangle_{R^0} \otimes |\text{dum}\rangle_{X^{00}} \otimes |1\rangle_{Y^{10}} \mapsto |1\rangle_{A_{\text{in}}} \otimes |2\rangle_Q \otimes |\text{dum}\rangle_{D^0} \\
|\text{dum}\rangle_{R^0} \otimes |0\rangle_{X^{01}} \otimes |\text{dum}\rangle_{Y^{00}} \mapsto |0\rangle_{A_{\text{in}}} \otimes |3\rangle_Q \otimes |0\rangle_{D^1} \\
|\text{dum}\rangle_{R^0} \otimes |1\rangle_{X^{01}} \otimes |\text{dum}\rangle_{Y^{00}} \mapsto |1\rangle_{A_{\text{in}}} \otimes |3\rangle_Q \otimes |1\rangle_{D^1} \\
|\text{dum}\rangle_{R^0} \otimes |\text{dum}\rangle_{X^{00}} \otimes |0\rangle_{Y^{01}} \mapsto |0\rangle_{A_{\text{in}}} \otimes |3\rangle_Q \otimes |1\rangle_{D^1} \\
|\text{dum}\rangle_{R^0} \otimes |\text{dum}\rangle_{X^{00}} \otimes |1\rangle_{Y^{01}} \mapsto |1\rangle_{A_{\text{in}}} \otimes |3\rangle_Q \otimes |0\rangle_{D^1}
\end{cases}
\tag{5.6}
$$

Since the global index constraint restricts V_A's practical input and output spaces to those sectors where exactly one index is equal to 1, it also defines a routed isometry. V_B and V_C are defined similarly.

The routed unitary W_A is defined as follows:

$$
W_A : \begin{cases}
|0\rangle_{A_{\text{out}}} \otimes |0\rangle_Q \mapsto |\text{dum}\rangle_{R^0} \otimes |0\rangle_{X^{10}} \otimes |\text{dum}\rangle_{Y^{00}} \\[4pt]
|1\rangle_{A_{\text{out}}} \otimes |0\rangle_Q \mapsto |\text{dum}\rangle_{R^0} \otimes |\text{dum}\rangle_{X^{00}} \otimes |1\rangle_{Y^{10}} \\[4pt]
|0\rangle_{A_{\text{out}}} \otimes |1\rangle_Q \mapsto |\text{dum}\rangle_{R^0} \otimes |0\rangle_{X^{01}} \otimes |\text{dum}\rangle_{Y^{00}} \\[4pt]
|1\rangle_{A_{\text{out}}} \otimes |1\rangle_Q \mapsto |\text{dum}\rangle_{R^0} \otimes |1\rangle_{X^{01}} \otimes |\text{dum}\rangle_{Y^{00}} \\[4pt]
|0\rangle_{A_{\text{out}}} \otimes |2\rangle_Q \mapsto |\text{dum}\rangle_{R^0} \otimes |\text{dum}\rangle_{X^{00}} \otimes |0\rangle_{Y^{01}} \\[4pt]
|1\rangle_{A_{\text{out}}} \otimes |2\rangle_Q \mapsto |\text{dum}\rangle_{R^0} \otimes |\text{dum}\rangle_{X^{00}} \otimes |1\rangle_{Y^{01}} \\[4pt]
|0\rangle_{A_{\text{out}}} \otimes |3\rangle_Q \mapsto |0\rangle_{R^1} \otimes |\text{dum}\rangle_{X^{00}} \otimes |\text{dum}\rangle_{Y^{00}} \\[4pt]
|0\rangle_{A_{\text{out}}} \otimes |3\rangle_Q \mapsto |1\rangle_{R^1} \otimes |\text{dum}\rangle_{X^{00}} \otimes |\text{dum}\rangle_{Y^{00}}
\end{cases}
\tag{5.7}
$$

The routed unitaries W_B and W_C are defined in a similar way. Finally, the routed unitary Æ is given by the following:

$$
\text{Æ}_F : \begin{cases}
|\psi\rangle_{R^1} \otimes |\xi\rangle_{D^1} \otimes |\text{dum}\rangle_{S^0} \otimes |\text{dum}\rangle_{E^0} \otimes |\text{dum}\rangle_{T^0} \otimes |\text{dum}\rangle_{K^0} \mapsto |\xi\rangle_{F_A} \otimes |1\rangle_{F_C} \otimes |\psi\rangle_{F_T} \\[4pt]
|\text{dum}\rangle_{R^0} \otimes |\text{dum}\rangle_{D^0} \otimes |\psi\rangle_{S^1} \otimes |\xi\rangle_{E^1} \otimes |\text{dum}\rangle_{T^0} \otimes |\text{dum}\rangle_{K^0} \mapsto |\xi\rangle_{F_A} \otimes |2\rangle_{F_C} \otimes |\psi\rangle_{F_T} \\[4pt]
|\text{dum}\rangle_{R^0} \otimes |\text{dum}\rangle_{D^0} \otimes |\text{dum}\rangle_{S^0} \otimes |\text{dum}\rangle_{E^0} \otimes |\psi\rangle_{T^1} \otimes |\xi\rangle_{K^1} \mapsto |\xi\rangle_{F_A} \otimes |3\rangle_{F_C} \otimes |\psi\rangle_{F_T}
\end{cases}
$$
$$\tag{5.8}$$

Note that the Grenoble process is an isometric process, with the overall output dimension greater than the overall input dimension (in particular, V is a routed isometry). The process can be made unitary in a natural way, by an extra a 2-dimensional ancillary qubit to the input of the Past and adding routed wires of dimension $1 + 2$ from the Past to each of the routed unitaries W, bearing the same index as the wire from the Past to the corresponding V. This makes the process symmetric in time. As a result, this increases the dimension of the Hilbert space of the sector carrying the message between the first and second agents from 1 to 2. In turn, this increases the dimensionality of the input space to the unitaries V, making the entire process unitary.

Note also that the Future cannot necessarily determine the relative order of the first two agents from their control and ancillary qubits F_C, F_A, if the third agent performs a non-unitary operation (because the order information encoded in the ancillary qubit relied on knowledge of the state of the message before the action of the third agent).

One peculiar feature of the Grenoble process is that the qubit that we have called the 'target qubit' – that is, the system that passes between the intermediate agents – plays a dual role. On the one hand, it is the 'message' that the agents receive. On the other hand, it also plays a role in determining the causal order. In particular, after it passes through the first agent, its logical state determines which agent receives it next. Thus if Alice comes first and wants to send the target qubit to Bob, she must send him the $|0\rangle$ state, but if she wants to send it to Charlie, she must send him $|1\rangle$.

Our reconstruction of the Grenoble process makes it obvious that this feature is not necessary to make the process consistent. Starting from the same routed graph,

one can easily define a variation on the Grenoble process, in which Alice is also given a second, 'control' qubit. This control qubit determines which agent comes second, leaving Alice free to send that agent whatever state on the target qubit she likes. Bob and Charlie can also be given their own qubits. Since this process can be obtained by fleshing out a routed graph whose validity we have already checked, it is immediate that this new process is also consistent. This illustrates a useful feature of our framework for constructing processes with indefinite causal order; namely, that variations on a process can be defined in a straightforward way, leading to a clearer understanding of which features of the original process were essential for its logical consistency, and which other features can be changed at will.

5.4.3 The Lugano process

In Section 5.4, we already introduced the Lugano process (also known under the names BW and AF/BW) as the seminal example of a unitary process violating causal inequalities. It was first presented as a classical process [86, 87], whose unitary extension to quantum theory can be derived in a straightforward way [59]. As we place ourselves in a general quantum framework here, we will primarily focus on this quantum version of the process; we note that the classical version can be obtained from the quantum one by feeding it specific input states and introducing decoherence in each of the wires of the circuit. This shows, more generally, that at least some exotic classical processes are also part of the class of processes that can be built through our procedure.

Indeed, we will show here how the (unitary) Lugano process can be constructed from a valid routed graph; this will provide an example of a process violating causal inequalities that can also be accommodated by our framework. In fact, we will derive a larger family of processes, defined by a same valid routed graph, and display how the Lugano process can be obtained as the simplest instance of this family. The other processes in this family share the basic behaviour of the Lugano process, but can feature, on top of it, arbitrarily large dimensions and arbitrarily complex operations.

The logical structure

Before we present the routed graph for the construction of the Lugano process, let us start with an intuitive account of the logical structure lying at the heart of it. This logical structure can be presented as a voting protocol involving three agents, in which each of the agents receives part of the result of the vote before having even cast their vote. Why this is possible without leading to any logical paradox, of the grandfather type, is the central point to understand.

In this voting protocol, each agent casts a vote for which of the other two agents they would like to see come last in the causal order. Alice, for instance, can either vote for Bob or for Charlie to come last. If there is a majority, then the winning agent

can both i) learn that they won the vote, and ii) receive (arbitrarily large) messages from each of the two losing agents. As for the two losers, each of them can only learn that they lost (i.e. no majority was obtained in favour of them), and they cannot receive any messages from the other agents. If no majority is obtained, then all agents learn that they lost, and none of them can signal to any other.

This voting protocol would have nothing surprising if it assumed that the winner learns of their victory and receives messages from the losers 'after' all the votes are cast. Yet in the Lugano process, the crucial fact is that Alice, for instance, learns whether she won, and (if she won) receives Bob and Charlie's messages, *before* she casts her own vote; and the same goes for Bob and Charlie. This sounds dangerously close to a grandfather paradox, since each agent contributes to an outcome that they might become aware of before they make their contribution. It seems likely that the agents could somehow take advantage of this system to send messages back to their own past, and decide what they do based on those messages, leading to logical inconsistencies.

Why this never happens – why, more precisely, the agents still have no way to send information back to themselves – can be figured out with a bit of analysis of the voting system. Indeed, Alice, for instance, finds herself in either of two cases. The first one is that she won: a majority 'was' obtained in favour of her. This means that she cannot send messages to either of the agents, since only the winner can receive messages. Nor can she signal to other agents by casting her vote: her victory implies that both Bob and Charlie voted for her, in which case her own vote is irrelevant to the outcome. Therefore, if Alice wins, then she cannot send any information back to herself via the other agents.

Alternatively, Alice could lose the vote. If so, then she cannot receive any messages from the other agents, so she has no hope of sending information back to herself through their messages to her. Therefore, if she wants to send information to herself, she will have to try to change the outcome of the vote in her favour (thus creating a grandfather-type paradox). But she cannot do this by simply changing her own vote, as there being a majority in her favour only depends on how the other agents vote. Nor can she make herself win by encouraging the other agents to vote differently: Alice can only send a message to (say) Bob if Charlie voted for Bob as well; and this last fact entails that, whatever Bob does, there will never be a majority in favour of Alice. Therefore, if Alice loses, she cannot send any information back to herself. For this reason, the Lugano process, despite conflicting with intuitions about causal and temporal structure, does not lead to any logical paradoxes, after all.

The routed graph

Of course, our description of the Lugano process so far has only been pitched at an intuitive level. The point of the routed graph that we will now present is precisely to formalise this intuitive description; while the validity of this graph – defined as
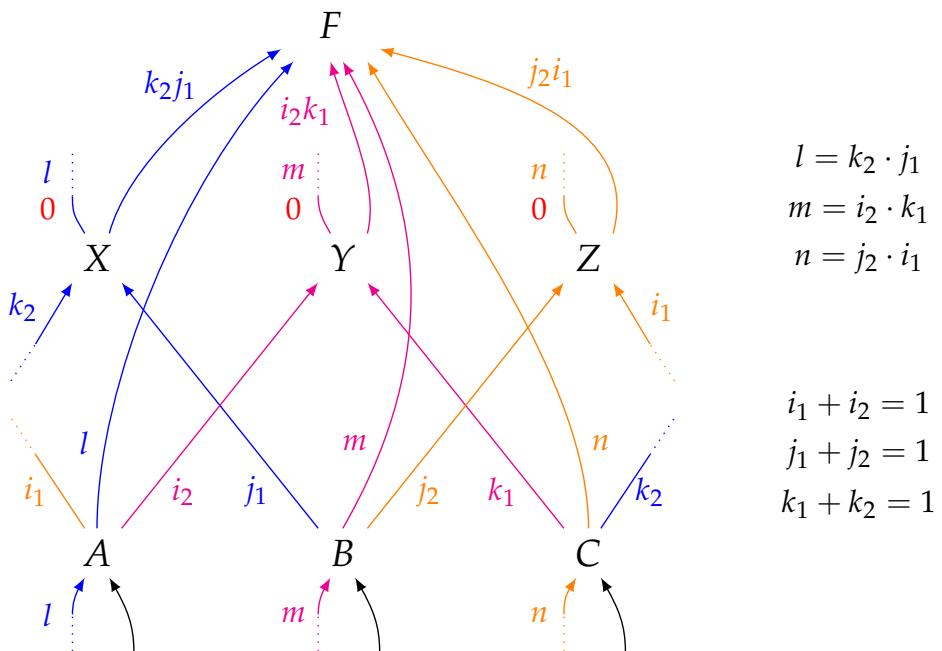
FIGURE 5.23: The routed graph for the Lugano process. To help intuition, we used different colours to denote the arrows that pertain to some particular agent (i.e. the ones whose indices encode the 'votes' or the 'vote result' for that agent). Each of the indices has only two possible values, 0 or 1. To reduce clutter, we have used arrows with dotted ends to avoid drawing all the arrows explicitly; pairs of dotted arrows with the same index are shorthand for a single unbroken arrow. For example, the pair of arrows with the index k_2 denotes a single indexed arrow $C \to X$.

$$\begin{cases} l = 0 \\ i_1 = 1 \\ i_2 = 0 \end{cases} \qquad \begin{cases} l = 0 \\ i_1 = 0 \\ i_2 = 1 \end{cases} \qquad \begin{cases} l = 1 \\ i_1 = 1 \\ i_2 = 0 \end{cases} \qquad \begin{cases} l = 1 \\ i_1 = 0 \\ i_2 = 1 \end{cases}$$

outputs

(+ values outside the practical outputs)

inputs $l = 0$ $l = 1$

A^0 A^1

'Alice loses'   'Alice wins'
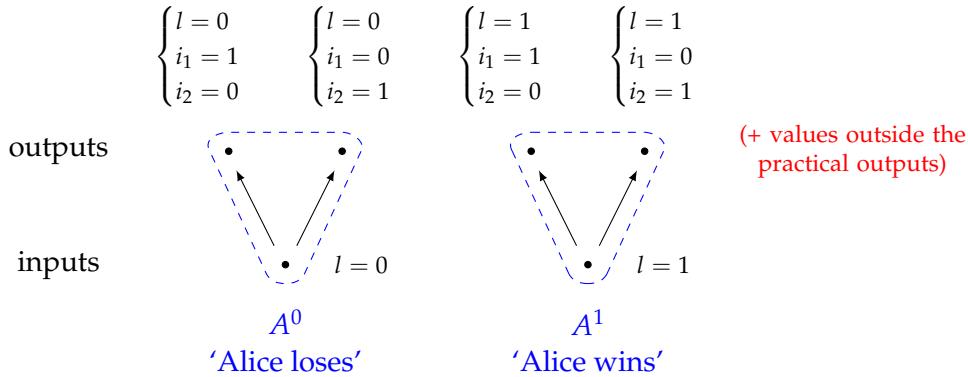
FIGURE 5.24: The branch structure of the route for node *A*. *B* and *C* are fully analogous.

the satisfaction of our two principles – will provide a formal counterpart to our argument that no logical paradoxes should arise from this protocol. Our routed graph is depicted in Figure 5.23.

In this routed graph, the nodes *A*, *B*, and *C*, representing the three agents, will be supplemented with three other nodes *X*, *Y* and *Z* which can be thought of – continuing with our metaphor – as 'vote-counting stations', in which the votes for each of the agents will be centralised and counted. *X* will deal with the votes for Alice, *Y* those for Bob, and *Z* those for Charlie.

Let us determine the routes in the graph and explain their meaning, starting with node *A*. The index *l* of the arrow going into *A* from its vote-counting station *X* indicates whether Alice won the vote (it has value 1 if she wins, and 0 if she loses). Furthermore, the indices i_1 and i_2 encode respectively whether Alice voted for Charlie or Bob, taking the value 1 when she votes for the corresponding agent. The index-matching of *l* ensures that Alice cannot change whether she wins or loses, while the floating equation $i_1 + i_2 = 1$ implies that Alice must vote for precisely one other agent. This leads to the route for *A* depicted in Figure 5.24. The route consists of two branches corresponding to Alice's victory or defeat, and a binary bifurcation choice representing her own vote in each case. The routes for *B* and *C* are fully analogous.

Now let us consider *X*, the vote-counting station for Alice. This node receives the index k_2, which tells us whether Charlie voted for Alice; and j_1, which tells us whether Bob did. It preserves these indices, sending them to the global Future, but also generates from them a new index *l* whose value is given by their product, $l = k_2 \cdot j_1$. This ensures that $l = 1$ just in case Alice wins the vote. The route for the *X* node has four branches, corresponding to the possible joint values of k_2 and j_1 (which we will denote $X^{k_2 j_1}$), and none of them include bifurcations. *Y* and *Z* work in the same way.

Finally, the 'global Future' node *F* just serves to channel out the remaining information. Since it receives all the distinct indices in the graph, its route is just given by the global index constraint. In other words, its practical input set of values is just
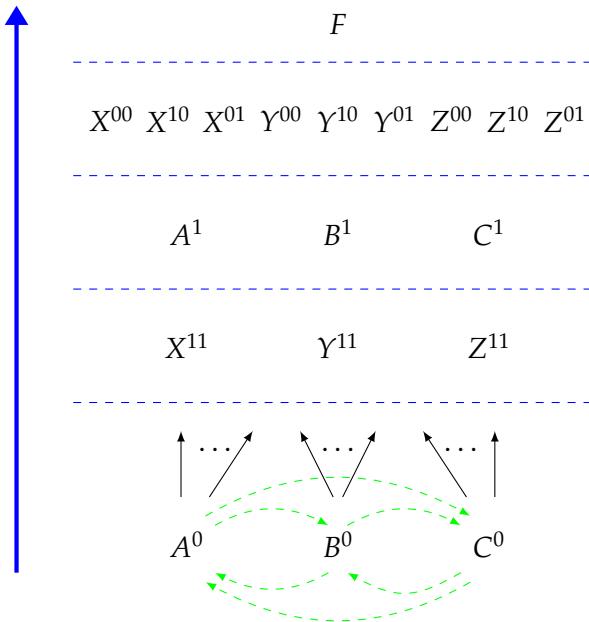
FIGURE 5.25: A simplified version of the branch graph for the Lugano process. We do not draw all the arrows, as this would create a lot of clutter and would be superfluous for our purposes of checking for cycles; we rather just organise the branches in layers, such that all unspecified arrows only ever go 'up' with respect to this partition.

the set of values permitted by the index-matching and the floating equations.

For the arrows $X \to A$, $Y \to B$, and $Z \to C$, the 0 value corresponds to a one-dimensional 'dummy' sector. The interpretation of this is once again natural: the messages are sent to an agent only if this agent won.

We can now check that the routed graph of Figure 5.23 satisfies our two principles. We start with univocality. The choice relation for this graph can be checked to be a function from the six binary bifurcation choices to the statuses of the branches. This function can be meaningfully presented in the following algorithmic way:

- Look at the votes of the losing branches (A^0, B^0 and C^0). If a majority is found in these votes (say, in favour of Alice), set the 'result' indices accordingly (in this case, $l = 1$, $m = n = 0$) and use the bifurcation choices of the losing branches (B^0 and C^0) to set the value of the votes of 'losers' (j_1, j_2, k_1, k_2); use the bifurcation choice of the winning branch (A^1) to define the value of the winner's vote (i_1 and i_2);

- If no majority is found, define $l = m = n = 0$ and use the bifurcation choices of the losing branches to set all votes.

- Now that the values of all indices in the graph have been fixed, derive which branches happened and which didn't.

Univocality is thus satisfied. Its time-reversed version can be checked to be satisfied as well: all bifurcation choices in the reverse graph are located in F, and they have the effect of fixing all indices to consistent joint values.

A simplified version of the branch graph is presented in Figure 5.25. We see that there *are* loops in the branch graph, specifically in its bottom layer; yet they are only composed of green dashed arrows. This entails that the routed graph of Figure 5.23 satisfies the weak loops principle, and is thus valid. This presence of weak loops is a signature of its causal inequalities violating nature.

The routed circuit
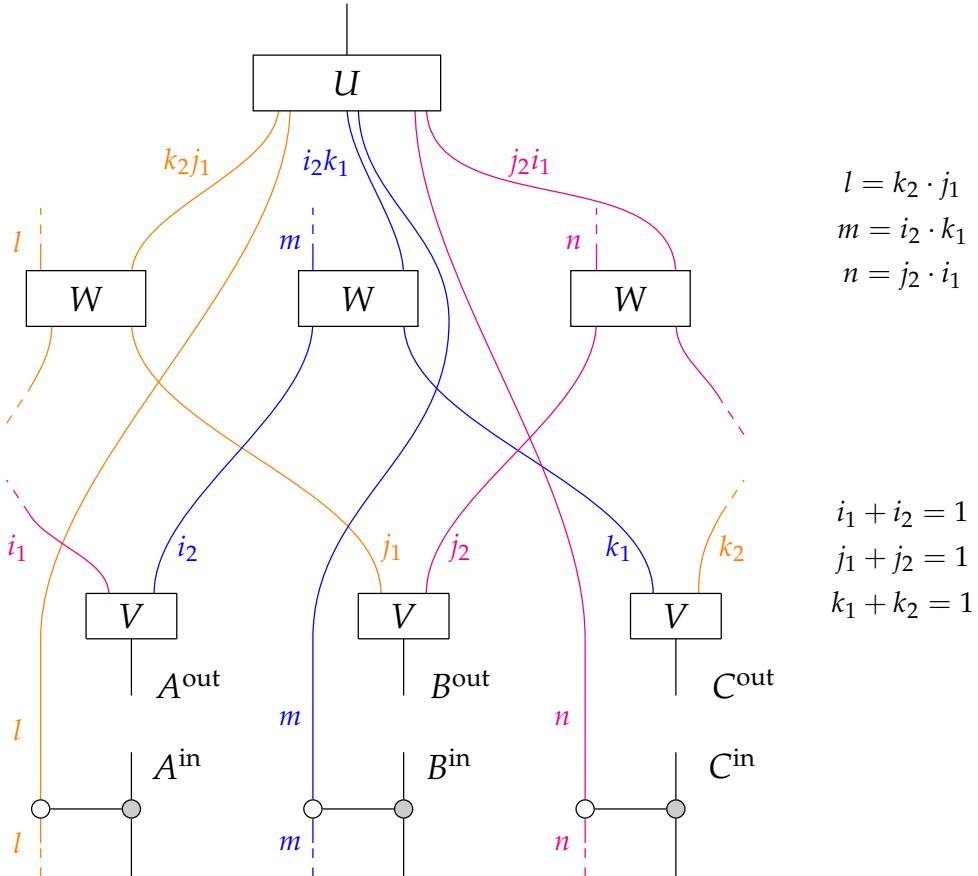
FIGURE 5.26: A routed circuit diagram for the Lugano process. We follow the same graphical conventions as in Figure 5.23. The gates at the bottom are CNOTs, controlled on the coloured wires.

We proved that our routed graph was a valid one, and therefore that any routed unitary circuit built from it will define a valid process. In particular, the Lugano process (as defined e.g. in equation (27) of Ref. [123]) is obtained by taking all sectors in all wires to be one-dimensional and by fleshing out the circuit as depicted in Figure 5.26. In this figure, V serves to encodes an agent's vote in the values of the outgoing indices; for example, the V above Alice's node can be written as

$$V := |i_1 = 1\rangle |i_2 = 0\rangle \langle 0| + |i_1 = 0\rangle |i_2 = 1\rangle \langle 1| , \tag{5.9}$$

where by $|i_1 = 1\rangle$ we denote a state in the $i_1 = 1$ sector. W sends the information about the value of its incoming indices to the Future, while also sending the information about the product of those values to the wire that loops back around to the Past. For example, the W above Alice's node is defined as

$$W := \sum_{x,y=0}^{1} |l = x \cdot y\rangle \, |(k_2, j_1) = (x,y)\rangle \, \langle k_2 = x| \, \langle j_1 = y| \, . \qquad (5.10)$$

Finally, U simply embeds its practical input space (defined by the global index constraint) into the global Future. Its precise form is irrelevant to our concerns, so we leave it out.

This shows how a paradigmatic unitary process that violates causal inequalities can be rebuilt using our method. We emphasise, however, that the Lugano process is merely the simplest example of a process obtained from fleshing out a routed circuit of the form of Figure 5.23; one could instead take this routed circuit to feature arbitrarily large dimensions (as long as the crucial sectors we specified remain one-dimensional), and fill it up with arbitrary operations (as long as they follow the routes). In other words, we have in fact defined a large *family* of processes that all rely on the same core behaviour as the Lugano process.

It is particularly worth noting that, while in the Lugano process the message sent to the winner is trivial (it is necessarily the $|1\rangle$ state), this family of consistent processes includes those where each losing agent can send arbitrarily large messages to the winner. Thus, the routed graph makes clear that the triviality of the messages in the original Lugano process is an arbitrary feature, that is not essential to the consistency.

5.5   Discussion

In this chapter, we presented a circuit formalism for indefinite causal order, based on the use of routes and on the exhibition of two principles, bi-univocality and weak loops, that single out the consistent connectivity structures. This ensures, and hence explains, the consistency of processes written using this circuit formalism.

Our circuit formalism can be used to represent a number of unitarily extendible processes. We explicitly constructed the quantum switch, the 3-switch, the Grenoble process, and the Lugano process. For each of these processes, the formalism also accommodates a large family of processes sharing the same connectivity – i.e. obtainable from the same routed graph. We expect that the other currently known examples of unitary processes that are built from classical processes analogous to Lugano can also be constructed using our method. Ultimately, we are led to the following conjecture.

Conjecture 1. *Any unitary process – and therefore any unitarily extendible process – can be obtained by 'fleshing out' a valid routed graph.*

Another fact pointing towards this conjecture is that bipartite unitarily extendible processes were recently proven [75, 85] to reduce to coherent controls of causal orders analogous to the switch, which can therefore be written as valid routed circuits. Our conjecture can be thought of as a tentative generalisation of this result to $\geq$ 3-partite processes. We expect that significant progress in this direction could be obtained if one were to prove another conjecture, that of the existence of causal decompositions of unitary channels in the general case (introduced in Section 2.3) [55].

This leads us to a limitation of our current results: they offer no systematic way to *decompose* a known process into a consistent routed circuit (except, in some cases, through a careful conceptual analysis of it). An important subject for future work, deeply related to the above conjecture, would be to come up with ways to supplement the bottom-up procedure presented here with a top-down procedure, in which one would start with a 'black-box' unknown process and extract a way of writing it as the fleshing-out of a valid routed circuit.

Another limitation is that we had no concern for the *physicality* of processes, i.e. for the question of whether and how they could be implemented in practice, using either standard or exotic physics. This was a conscious choice on our part, as we wanted to rather focus on the question of their logical *conceivability*. However, we expect that our way of dealing with the latter question might, through the clarifications and the diagrammatic method it provides, pave the way for work on possible implementations or on physical principles constraining them.

An important consequence of our work is that it shows how at least a large class of valid quantum processes can be derived from the sole study of *possibilistic* structures, encapsulated by routes. These possibilistic structures impose constraints on quantum operations, but there is nothing specifically quantum about them; they could be interpreted as constraints on classical operations as well. This adds to the idea, already conveyed by the discovery of classical exotic processes, that the logical possibility for indefinite causal order does not always arise from the specifics of quantum structures. If our above conjecture turned out to be true, this would warrant this conclusion for any unitary and unitarily extendible process, whose quantum nature is nothing more than coherence between the branches of an equally admissible classical process.

By contrast, some non-unitarily extendible processes, such as the OCB process [18, 59], appear to feature a more starkly quantum behaviour in their display of indefinite causal order. This can be seen for example in the fact that the violation of causal inequalities by the OCB process relies on a choice between the use of maximally incompatible bases on the part of one agent. A more quantitative clue is the fact that the OCB process saturates a Tsirelson-like bound on non-causal correlations [124]. It is therefore unlikely that such processes could be built using our method, as routes do not capture any specifically quantum (i.e. linear algebraic) behaviour. In particular, the display of a unitary process with OCB-like features would probably

provide a counter-example to our conjecture.

In the course of the presentation of the framework and of the main examples, we commented on the fact that the presence of (necessarily weak) loops in the branch graph were associated with the violation of causal inequalities: processes showcasing (possibly dynamical) coherent control of causal order, and therefore incapable of violating causal inequalities [84] – such as the switch, the 3-switch and the Grenoble processes – featured no such loops; while the Lugano process, which does violate causal inequalities, had loops in its branch graph. This leads us to the following conjecture.

Conjecture 2. *The skeletal superunitary corresponding to a valid routed graph violates causal inequalities if and only if its branch graph features (necessarily weak) loops.*

Proving this conjecture would unlock a remarkable correspondence between, on the one hand, the structural features of processes, and, on the other hand, their operational properties. An interesting question is how this would connect to (partial) characterisations of causal inequalities-violating processes via their causal structure [125].

Our work facilitates a transition from a paradigm of defining processes with indefinite causal order one by one and checking their consistency by hand, to one of generating large classes of such processes from the study of elementary graphs, with their consistency baked in. In that, it follows the spirit of Ref. [84], with more emphasis on the connectivity of processes and on the formal language with which one can describe the consistent ones. Another difference is that the framework presented here also allows us to build at least some of the unitary processes that violate causal inequalities [126].

A natural application would be to build and study new exotic processes using our framework; we leave this for future work. More generally, the fact that our rules for validity only rely on the study of graphs decorated with Boolean matrices opens the way for a systematic algorithmic search for instances, using numerical methods.

A final feature of our framework is how, through the use of graphical methods and meaningful principles, it makes more intelligible, and more amenable to intuition, the reasons why a process can be both cyclic and consistent – a notoriously obscure behaviour, especially in the case of processes violating causal inequalities. Our two rules for validity, however, are still high-level; further work is needed to investigate their structural implications. This could eventually lead to a reasoned classification of the graphs that satisfy them, and therefore of (at least a large class of) exotic processes.

Chapter 6

Conclusion and outlook

At the age of twenty, he had assumed himself free from the routine or prejudice that hamper our actions and set blinkers on our intelligence, yet his life had been spent in acquiring penny by penny this freedom which he had thought entirely his from the outset.

Marguerite Yourcenar, *The Abyss*.

6.1   Summary

In this thesis, we extended the framework of quantum circuits in order to capture coherent control and indefinite causal order. Our extension relied on the incorporation of *sectorial constraints*, restricting how some of the dynamical maps are allowed to connect input sectors to output sectors. We formalised these constraints as *routes*, living in the theory of relations (or Boolean matrices). This yielded *routed quantum circuits*.

As it turns out, this basic alteration leads to a dramatic extension of the range of scenarios that the framework can describe. For example, one of its simplest instantiations, only involving a one-dimensional sector and a *d*-dimensional one, is sufficient to formalise and study the base case of coherent control, a task that had been at the centre of an imbroglio between theory and experiments, due to the shortcomings of standard circuits. More involved cases – whose description requires little effort, due to the straightforward way in which the framework scales up – then span the whole spectrum of quantum control; in fact, routed quantum circuits could retrospectively be thought of as a definition of the form of arbitrarily manifold quantum control.

Furthermore, we showed how routed circuits can be used to express coherent control of the causal order of operations, whose description had so far remained at a rudimentary level in terms of intuitiveness, pliability, and scalability. The route structure has the ability to encode in a nutshell the core behaviour of processes with such indefinite causal order. In particular, it allows one to readily check the processes' consistency, a particularly crucial task in this context, as feedback loops

generically lead to inconsistencies. The range of unitary scenarios that routed quantum circuits encompass extends to at least some of the *non-causal* ones, in which the order is itself decided in a global, acausal way.

6.2 Current limitations of the framework

We stop boasting for a minute and consider the shortcomings of the framework as it stands.

6.2.1 Non-compositionality of the physical maps

One shortcoming is that, even in the case of an acyclic structure, it is necessary to check conditions on the route structure in order to ensure that the whole circuit preserves physicality (i.e. yields a physical map when filled with physical maps): this can be done either through constructing the circuit via well-behaved compositions (in the sense of Section 3.1.3); or, in the index-matching case, by checking the simpler global rules described in Section 3.4; or by checking the global condition of bi-univocality (Section 5.3), which also has to be satisfied in the acyclic case (and is in fact then sufficient, as weak loops is trivially satisfied). In any case, merely having an acyclic structure is not a sufficient condition for a routed circuit to be suitable.

We already mentioned this shortcoming in Chapter 3's footnote 1. As we stated there, we believe that there is no way around this difficulty when dealing with quantum control, so that the best we could do was to keep it to its minimal level, and to provide the structural tools to manage it in general. The reasons for this belief in the inevitability of some level of 'non-compositionality' of the physical maps have a lot to do with having spent generous amounts of time unsuccessfully trying to do away with it. Let us however try to spell out the intuitions we developed as to why this could not work out.

The non-compositionality is essentially due to how we allowed the route to specify a 'practical' part of the routed maps' input and output spaces (see Section 3.1.3). This led to the fact that composing routed maps in sequence could modify their practical input and output spaces, sometimes in such a way that the map obtained does not describe the whole information flow between these spaces, because of 'holes in the racket'. A simple example is the composition of routed isometries (λ, f) and (μ, g), where the structure of the routes λ and μ is

$$\begin{array}{cc} \mu \uparrow & \\ \lambda & \searrow \nearrow \\ & \cdot \end{array} \tag{6.1}$$

in which one can then see that in $(\mu \circ \lambda, g \circ f)$ we have a hole in the racket, in the sense that some of the information flow from its practical input space is lost. The

condition for suitable composition expressed in Theorem 3.1.2 is there precisely in order to exclude such cases.

A natural criticism would be to argue that we had it coming when we started reasoning in terms of somewhat flexible practical input and output spaces; if we had hardcoded the input and output spaces instead, none of these shenanigans would be possible, and surely the theory would recover full compositionality. Our reply to this criticism is that this alternative method would itself lead to a flurry of issues – related, this time, to parallel composition – among which one would eventually find the very issue we tried to move away from in the first place.

To see this concretely, let us go back to our paradigmatic example of a routed circuit, the one for the superposition of trajectories, presented in (3.8):

$$
\begin{array}{c}
\omega_{ln} \quad \boxed{U^\dagger} \\
\delta^l_k \quad \boxed{V_1} \qquad \boxed{V_2} \quad \delta^n_m \\
\omega^{km} \quad \boxed{U}
\end{array}
\tag{6.2}
$$
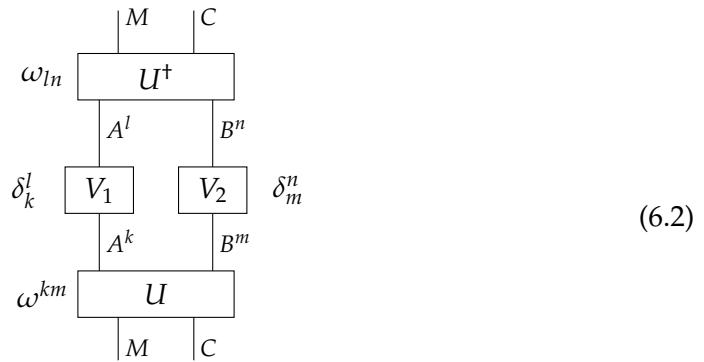
In our framework, the middle layer's map is $(\delta \times \delta, V_1 \otimes V_2)$, whose practical input space is $\bigoplus_{i,j} \mathcal{H}^i_A \otimes \mathcal{H}^j_B$. Yet it is composed with (ω, U), whose practical output space is $\tilde{\mathcal{H}}_{A,B} := \bigoplus_{i,j} \omega^{i,j} \mathcal{H}^i_A \otimes \mathcal{H}^j_B = \mathcal{H}^1_A \otimes \mathcal{H}^0_B \oplus \mathcal{H}^0_A \otimes \mathcal{H}^1_B$. Thus we see once again how our framework deals flexibly with practical spaces (in a harmless way here, as the conditions for Theorem 3.1.2 are satisfied). This also relates to the discussion of Section 3.2 on how the notion of accessible space is a contextual one.

The alternative method mentioned above would prescribe to avoid this flexibility and to somehow hardcode the middle layer's input space to be $\tilde{\mathcal{H}}_{AB}$ as well. Because this middle layer is a parallel composition of two maps whose input spaces are obviously $\mathcal{H}_A$ and $\mathcal{H}_B$, this hardcoding can only happen as a part of the procedure by which we compose them. In other words, we are led to the idea that there should be an 'ω' tensor product that takes the individual maps and combines them into one whose input space is specifically $\tilde{\mathcal{H}}_{AB}$. More broadly, it appears that in a general framework, we would need to have at our disposal a whole family of parallel compositions $\otimes_\omega$ with which to combine individual maps in order to hardcode any set ω of sectorial correlations between their input spaces.

Issues start arising when we try to check – or even define – the structural properties of these families of parallel compositions. A few examples are:

- Associativity: should $((\lambda, f) \otimes_\omega (\mu, g)) \otimes_{\omega'} (\nu, h)$ be equal to $(\lambda, f) \otimes_\omega ((\mu, g) \otimes_{\omega'} (\nu, h))$?

- Distributivity: does $\otimes_\omega$ distribute over the sequential composition $\circ$, and if yes, in which sense?

- Relationship with the dagger: we defined our parallel products as hardcoding a suitable input space for the product map. But what will its output space be? Generically, it will depend on the maps' routes themselves, which is already problematic from a structural point of view. And how will we provide rules for computing $((\lambda, f) \otimes_\omega (\mu, g))^\dagger$?

- Physicality: some physical maps cannot be meaningfully composed with a $\otimes_\omega$ (e.g., in our main example, if we had taken f and g to have 'full' routes allowing for connections between all sectors, then composing them with $\otimes_\omega$ would not have been meaningful). When is it possible? How does that play with the two previous issues?

In particular, the last point is nothing but another avatar of the issue we tried to avoid, namely that some compositions are not legal and that non-trivial rules will have to be spelled out in order to specify which. Adopting the alternative method simply led us to encounter this problem with the parallel, rather than the sequential, composition. We are thus left with a method in which our original issue is still present, together with numerous new ones.

It is for that reason that we believe the issues with non-compositionality of physical maps are, to some extent, unavoidable. We would gladly welcome any worked-out framework that would prove this belief wrong, as this non-compositionality is unquestionably an inconvenience.

6.2.2   Opacity of the diagrammatic notations

The goal of diagrammatic notations should be to provide as much intuition as possible to the reader. In that respect, our notations seem to only go halfway: they allow one to represent the connectivity of the factorial structure, and provide some intuition about the behaviour of the sectorial structure (in particular whenever index-matching is used); but in general the latter remains somewhat cryptic, relying on abstract symbols (the floating routes) or equations (when using global index constraints) that the reader has to parse through. Accordingly, checking the circuits' consistency, even though considerably simpler than before, remains a non-trivial task.

Progress on the design of further intuitive notations seems to us an achievable prospect in the near future, especially now that the semantic aspects have been cleared out. An idea would be to focus on graphically representing bifurcations (as introduced in Chapter 5). In general, the challenge is to represent, in a same diagram, both the factorial structure (i.e. the connectivity) and the sectorial structure (i.e. the routes' specification, as represented for example in Figures 5.20 or 5.25). This is related to the general issue of the design of wieldy diagrammatic notations for both monoidal structures at once in a bimonoidal category.

On that front, the diagrammatic notations recently put forward in the frameworks we presented in Section 2.4.4 could provide a valuable source of inspiration.

In particular, those of many-worlds calculus [102] bear some similarity with the notions used in this thesis, even though they were not used with the same goals so far. It would be natural to see how the two can be joined.

6.2.3 Absence of a diagrammatic calculus

A related drawback is that our routed circuits provide no diagrammatic calculus, except for some anecdotal cases. More precisely, because they arise from a †-compact category, routed circuits lend themselves to the basic calculus of circuit and string diagrams, corresponding to equivalence under distortion of the diagrams, just as standard quantum circuits did. But beyond this, no equalities between diagrams can be inferred solely from their form – except in some cases linked to the use of Kronecker deltas, as in (3.17).

More precise diagrammatic notations, as motivated above, could help unlocking non-trivial equalities between diagrams. In any case, this is a point on which the minimality of routed circuits as an extension of quantum circuits, which we mentioned already, could help. Because routed circuits contain exactly the additional information required to specify the crucial features of the scenarios at hand (namely, the sectorial constraints) and to check them for consistency, nothing prevents from adjoining to them further overlays of structural features and/or diagrammatic notations, more suitable to one's needs in one context or another.

For instance, it is conceivable that some version of PBS-calculus [96, 97] or of LOv calculus [98] could be defined as living on top of an underlying routed circuit structure, to describe quantum-optical scenarios. In such a framework, the remarkable computational power of these calculi would simply be supplemented with the information encoded by the routes – in particular with the safety they provide in terms of preservation of physicality. The same could be tried with many-worlds calculus [102] or even with ZX-calculus [11, 127].

6.2.4 Valid yet not provably valid routed graphs

A limitation of the conditions for the validity of routed graphs described in Section 5.3 is that they are sufficient, but not necessary. In other words, any routed graph satisfying them defines a valid skeletal supermap, but some routed graphs define a valid skeletal supermap despite not satisfying them (and specifically, not satisfying the weak loops condition).

An example is the routed graph that one would obtain if one wanted to check the consistency of the circuit of Figure 5.1 for the switch without pruning it into the simplified circuit of Figure 5.2 beforehand. This routed graph would have the form

$$\text{(6.3)}$$
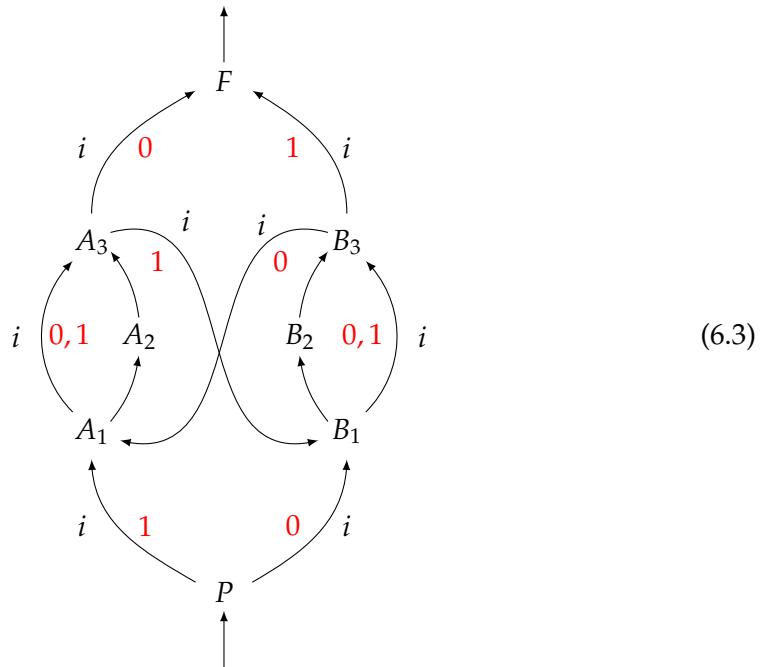
and yield the branch graph

$$\text{(6.4)}$$
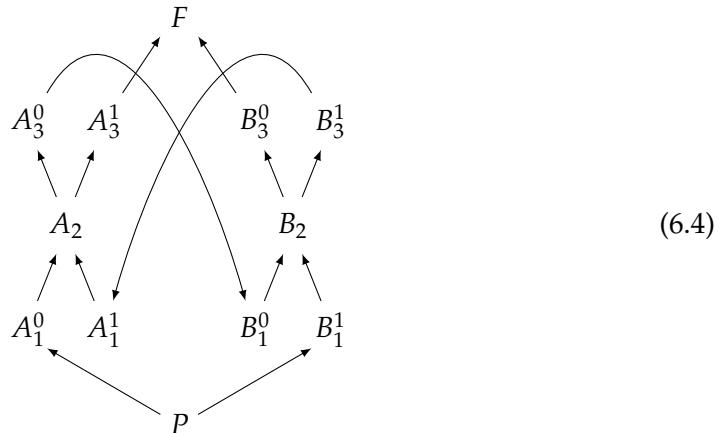
which features solid loops. (We have not represented the dashed arrows; they simply come from P and go to F.) Yet the skeletal supermap corresponding to (6.3) is valid, as it can be directly obtained from a partial fleshing-out of that of Figure 5.2.

    We can see that the issue here is due to 'fake' paths. More precisely, the presence of A_2 induces a path from A_1^1 to A_3^0 in the branch graph, eventually leading to a loop; yet it is not hard to get convinced that this path is a 'fake' one, because A_1^1 and A_3^0 are incompatible branches: they never happen together. Once this is taken into account, one can get convinced, at least morally, that the routed graph indeed could not lead to any paradox.

    This state of affairs is still an annoyance, however, as it means that our method for checking routed graphs might miss valid ones. Accordingly, somebody naively considering (6.3) cannot be assured that it yields a valid superchannel, except by realising that it can be obtained from the simpler, and provably valid, Figure 5.3.

Fortunately, such situations seem to arise only when the routed graph becomes 'too detailed' (as is the case for (6.3) compared to Figure 5.3), although there is no mathematical certainty of this.

A conceivable solution would be to make our conditions for validity weaker, by stating that a loop in the branch graph should not be considered harmful in case it includes at least two incompatible branches. This would require an amendment of the proof of Theorem 5.3.1 to generalise it to this case; this would be a non-trivial task, as the proof relies on the definition of a partial order between the branches, which would not be readily available in this case. It is not impossible that such a generalised theorem would in fact turn out to be false, due to some subtle counter-examples. In any case, the question would require further research.

6.3 Other work on routed circuits

We have carried out further work on the subject of routed circuits, but have not included it in this thesis. We briefly review it, focusing on the aspects that are relevant to our subject of interest.

6.3.1 A categorical generalisation: composable constraints

A question of interest from a structural point of view is to pin down what exactly, in the structural properties of quantum theory, allows us to derive a theory of routes, and to which extent this strategy is generalisable to other theories, or to other properties of quantum theory. The framework of *composable constraints* [4] aims at tackling this question.

As discussed in this paper, at an abstract level, what we did with routes is display a theory **Con** of constraints on a theory **C**, that features compositional structure compatible with its interpretation as constraints: for instance, if f (living in **C**) follows the set of constraints λ (living in **Con**), and similarly g follows μ, then $g \circ f$ follows $\mu \circ \lambda$, etc. This is characterised by the existence of a lax functor from **Con** into the powerset category of **C**. Having a composable constraint allows us to build a constrained category, in which **Con** and **C** live side by side.

In particular, Ref. [4] discusses the ways in which one can generically build a constraint category **Con** by leveraging on the existence of some standard structure of **C**. A typical example is that of categories enriched over commutative monoids; intuitively, this corresponds to process theories that admit a notion of 'summing processes together'. Such theories always admit a theory of sectorial constraints encoded by (finite) relations, with the constraints precisely restricting the behaviour of maps with respect to this summation structure. Routes as presented in this thesis correspond to the case in which **C** is the theory of finite-dimensional Hilbert spaces and linear maps.

Interestingly, this generalises to provide other interesting examples of theories of composable constraints, especially in the case of quantum theory. In particular,

a connection can be made back to the study of quantum theory's causal structure, which we briefly presented in Section 2.3. Indeed, finite relations can be used to encode constraints in a more general case than categories enriched over commutative monoids: they can be used over any semicartesian category, i.e. any theory with only one effect per object. As it turns out, applying this construction to the theory of quantum channels (which indeed has only one effect per object, namely the discarding map) yields a theory in which relations now encode constraints on the possible signalling between input and output factors of a channel.

This means that we managed to spell out the reason for the deep analogy between the study of the *sectorial* structure of quantum theory – described by sectorial constraints –, and that of its *factorial* structure – described by signalling constraints. Namely, they arise from the fact that two of the process theories used in quantum theory are each semicartesian with respect to a parallel composition: complex linear maps are semicartesian with respect to the direct sum – allowing us to describe sectorial constraints –, while quantum channels are with respect to the tensor product – allowing us to describe signalling constraints. This also entails that one can define a theory in which 'routes' would be used to encode signalling constraints rather than sectorial ones. An interesting prospect is that of defining 'routes' that would capture both at once; this would be a significant step in capturing jointly the two important monoidal structures of quantum theory.

Finally, Ref. [4] discusses the time-symmetry of such constraints, and links it to the question of whether they are intersectable, i.e., intuitively, whether they can be considered as sets of logically independent constraints. This yields interesting insights into the reason for the atomicity (as defined in Section 2.4.3) of the signalling structure for unitary channels, and its failure in the case of general quantum channels.

6.3.2 A study of the causal structure of routed circuits, with an application to the switch

The other recent work on routed circuits [5] also branches back to the study of quantum causal structures, from which they arose in the first place. In this work, the question is whether one can give a notion of the causal structure of a scenario in which sectorial constraints are present, and whose formalisation is consequently a routed circuit rather than a standard one.

Interestingly, not only is this possible – generalising the results of Ref. [69] –, but the additional structure described by the sectorial constraints allows for a fine-graining of this causal structure, in which the causal relations are defined not between factors, but between individual sectors, together with a 'which-sector' information. This type of analysis is applied to the case of recent implementations of the quantum switch: first, it is shown that these implementations admit a model in terms of a more general 'routed switch', defined as a routed superchannel in the sense of Section 4.6; second, it is shown that even though the coarse-grained causal

structure of the routed switch is cyclic, its sectorised causal structure is acyclic. This warrants the conclusion that the implementations realise indefinite causal order in a weak sense.

This work carries further the program of studying the properties of scenarios that feature sectorial constraints. It further demonstrates the relevance of routed circuits in this context, as they provide the formal basis for a general study of these scenarios. In particular, it shows that these scenarios are particularly well-behaved, in the sense that they allow for causal modelling, and even for a fine-grained version of it. With the routed switch, it displays an important example of a non-trivial and physically relevant routed superchannel.

It also shares some similarities with the considerations of Chapter 5. The routed switch, for example, is nothing else than the bipartite routed superchannel obtained by filling up the past and future nodes in the skeletal superchannel Figure 5.2. More generally, there is an obvious connection between the way in which Ref. [5] fine-grains the causal structure of a routed superchannel into one relating its branches, and the way in which we infer and study a branch graph from a routed graph. In a broad sense, Ref. [5] and our Chapter 5 go in opposite directions: the first starts from a valid superchannel and infers its causal structure, while the second starts from a certain compositional structure and infers the validity of the superchannel from it.

However, there is a crucial difference to keep in mind: while Ref. [5] discusses the *causal* structure, our Chapter 5 starts from a *compositional* structure. That the relationship between the two is a subtle matter is what led, in the case of unrouted unitary channels, to the study of causal decompositions, which we presented in Section 2.3. This relationship should also be studied further in the case of routed superchannels. In particular, while the 'causal structure $\implies$ compositional structure' direction is still out of reach (remaining a conjecture even in the unrouted case), the 'compositional structure $\implies$ causal structure' appears a manageable one. The idea would be to study the causal structure of the skeletal superchannel corresponding to a (valid) routed graph, and to see how it can be inferred from the properties of this graph. Our expectation is that the sectorised causal structure will look closely like the branch graph, although it might be slightly different in some cases.

6.4 What's next?

We end this thesis with a discussion of some of the research directions that it opens up.

6.4.1 Routed circuits as a formal type structure

In Section 2.4.4, we mentioned the recent flurry of research into the type structure of higher-order theories. As we remarked, a drawback of the existing typings is that they are not detailed enough to yield a constructive way in which exotic superchannels (such as the switch) can be obtained by composing the slots they are

built from. Our Chapter 5 precisely provides such a way. An interesting research direction would be to formalise these results into a well-defined type structure, that would extend and complete the work undertaken in the existing literature.[1]

A particular challenge is that this will mean formally including routes into processes' types.[2] This will very probably make the type systems much richer compared to their (already non-trivial) current state. The interaction of the 'route-types' with the rest of the structure of higher-order process theories (e.g. their *-autonomous structure) is in particular an important subject of enquiry.

Once this first step is achieved, it is conceivable that our Theorem 5.3.1 could be framed as the existence of an exotic composition linking together several input processes of certain types, whenever these types satisfy some formal conditions, which would be translations of our two conditions for the validity of routed graphs. Successfully pinning down these non-trivial compositions in terms of types would help making our results more palatable in structural terms. Note that all this work could also be carried out within the parallel research program in which higher-order theories are characterised in terms of their intrinsic structure, rather than as constructions over a first-order base theory [94, 95].

6.4.2   Studying the class of route-generated superchannels

In Chapter 5, we implicitly introduced a new class of superchannels: the ones that can be obtained by fleshing out a valid routed graph. We conjectured that this class is equal to that of unitarily extendible superchannels. But even if this conjecture turned out to be false, or too difficult to prove, this new class of 'route-generated superchannels' would still be an interesting one to explore. This is because, in contrast to most classes of superchannels, which are defined in terms of their phenomonological properties (and whose structure therefore remains obscure), the supervised way in which route-generated superchannels are built grants considerable leverage to study their features in detail.

Our Conjecture 2 is a first instance of this: while the structural characterisation of causal inequality violations in superchannels seems way out of reach in the general case, it looks like a manageable goal once one restricts one's attention to route-generated superchannels. Similarly, characterising the superchannels that are or are not QC-QCs would be a natural task within this class. As we argued in Section 2.4.3, we more generally believe that the study of most questions concerning the structure and properties of superchannels – e.g., concerning their physicality, the advantages

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[1]Some confusion might arise from the fact that Ref. [91] already studies the consequences of the existence of additive structure in the base category: this might lead to thinking that sectorial constraints have been included in the framework already. However, the additive structure considered in Ref. [91] only corresponds (in the context of quantum theory) to *incoherent mixtures* of processes, while the point of sectorial constraints is, in broad terms, to model the *coherent superpositions* of processes. This is closely related to our discussion in Appendix A.2.

[2]This would represent a formal translation of the remarks we make in Appendix A.1, where we note that routes should morally be understood as types, even though in the current theory they are not properly framed as such.

they yield in physical, computational or communicational tasks, their certification, their possible implementations – will greatly benefit from the intuition that route-generated superchannels allow. We see Ref. [5] as a first instance of these beneficial upshots: improved clarity, graphical intuition, scalability, fine-grained conceptual architecture, etc.

Another related line of research would be to take advantage of the relative simplicity of routed graphs to both generate and study them using numerical methods. A computer program could for instance look through the space of all routed graphs of a certain size, single out the valid ones, and check their properties, possibly yielding interesting new examples, or classes of examples, of exotic processes. This would benefit from making our conditions easier to check numerically; their current form, more aimed at human intuition, is probably not the most efficiently checkable by computers.

6.4.3 Other cases of sectorial constraints

Finally, besides the applications to indefinite causal order, we believe that there are many scenarios in various parts of the quantum-theoretical literature that implicitly feature sectorial constraints, and to which our framework could be fruitfully applied. This belief stems from the mathematical fundamentalness and ubiquitousness of C*-algebraic structures, whose proper representation in the generic case can only be obtained through the use of routes, as we argued in Section 2.2.2. Framing these scenarios in terms of routed circuits has the potential to clarify their features and properties, in a similar way to what we achieved in the case of coherent control in Chapter 4.

An example of a scenario to which our framework could be applied in the future is the del Santo-Dakić (dSD) protocol [128–130], in which a controlled dephasing between the vacuum and the one-particle sectors allows agents to achieve 'two-way communication with a single particle' in a way that would not be possible classically. It has already been argued [131] that the original presentation of the dSD protocol was misleading, in the sense that it did not acknowledge explicitly the crucial importance of the vacuum sector of the agents' actions. In our view, routed circuits (together with their causal analysis provided by Ref. [5]) would be the proper tool to provide a more formal account of dSD, that would clarify its definition and the resources it features (in the spirit e.g. of Ref. [49]). In broad terms, this is due to the fact that the main challenge is to take into account the vacuum sectors while maintaining the crucial 'one-particle only' assumption, a task for which sectorial constraints and correlations are the perfect tools.

Another example is the Aharonov-Bohm effect [132], which also relies on the superposition of a particle's trajectory. A particularly intriguing possibility for us is to apply our framework to the very active field of quantum reference frames, which also deals with superpositions of particles' positions. Quantum reference frame transformations, in particular, might be understood as routed unitaries, linking the

description in which a given particle is in superposition to the one in which it is localised.

More generally, our intuition is that the presence of any physical rule of conservation of a quantity (e.g. energy, centre-of-mass position, momentum) will generically translate, at the abstract informational level, into sectorial constraints corresponding to sector-preservation with respect to the eigenspaces of the corresponding observable. 'Fundamental' conservation rules (in the sense that they arise not from some technological or methodological limitations, but from the nature of the physical situation at stake) are an especially attractive prospect.

It would be valuable to explore how sectorial constraints are connected to, and possibly shed light on, superselection rules [133] – which are indeed central features of the subjects we just mentioned. It seems to us, from a very preliminary investigation, that a major difference lies in the fact that superselection rules are traditionally taken to result in the loss of all coherence between the sectors, while sectorial constraints allow for this coherence to be present. That coherence can be preserved and recovered in later transformations is also at the heart of the more recent approaches to quantum reference frame transformations, which reinforces our belief in the existence of a deep connection between the two subjects.

A framework is not merely a passive architecture in which to allot pre-available objects of study. To a large extent, the framework *defines* what is an appropriate object of study in the first place; its overhanging presence channels the researcher's intuition into spotting and catching instances of deemed-proper objects, while discarding or simply not minding other candidates, regarded as ill-defined. It is commonplace in the history of science to observe that the advent of a new framework led to the sudden dicovery of applications and phenomena that, in retrospect, had been standing in plain sight all along. Quantum circuits themselves have been an example of this. Our hope is that routed quantum circuits – and specifically their incorporation of systems whose dynamics suffers sectorial constraints – could, at their modest scale, achieve the same.

Appendices

That, however, of which I am master and knower, is the brain of the leech: that is my world! And it is also a world! Forgive it, however, that my pride here findeth expression, for here I have not mine equal.

Friedrich Nietzsche, *Thus Spoke Zarathustra*.

Appendix A

Appendices for Chapter 3

A.1 Comments on the conceptual role of routes

In this Appendix, we will provide a few comments on the conceptual role of the route in a routed map. This conceptual role can be understood by appealing to the notion of *type*. Usually, specifying the type of a linear map f means declaring its input space and its ouput space. Thus the type of a map is a structural piece of data which is prior to the specification of this map itself, with which the map itself is consistent, and which gives information about the ways in which this map can be composed: for instance, f and g can be composed only if f's output space matches g's input space. In a routed map (λ, f), λ should be morally understood as having the role of an *additional type* for f, that comes as a supplement to the declaration of its partitioned input and output spaces.[1] This is indeed the case once one restricts to the theory of practical isometries or to that of routed quantum channels: routes – and not solely input and output spaces – have to be taken into consideration to determine which maps can be meaningfully composed.

That routes play the part of an additional type should also shed light on the seemingly disturbing fact that a given linear map f can be compatible with several different routes,[2] and on the natural question one can then ask: 'what is the difference between (λ, f) and $(\tilde{\lambda}, f)$?'. Our comments entail that this is essentially a question about the meaning that is to be ascribed to a modification of the type assigned to what is, morally, the same map. In fact, similar questions about the meaning of a type change can also arise for non-routed linear maps. Indeed, a same given linear map can also, while morally staying the same map, be ascribed a variety of output spaces (basically any space of which its 'actual' output space is a subspace). In both this case and the case of a route change, the type change does not essentially modify the map, but it does modify our capacity to hold structural statements about it, and, in particular, to state what it is meaningful to compose it with.

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[1] Let us stress, however, that this is a *moral* account of routes, aimed at clarifying their conceptual role. From a purely formal point of view, the types of routed maps solely consist of their partitioned input and output spaces.

[2] If f follows λ, then f also follows any $\tilde{\lambda}$ such that $\forall k, l, \tilde{\lambda}_k^l \geq \lambda_k^l$.

A.2 Connection with the CP* construction and other strategies

In Sections 2.2 and 2.3, we showed that standard quantum circuits (i.e. those interpreted in either **FHilb** or CPM [**FHilb**]) could not be used to provide an adequate description of superpositions of trajectories or causal decompositions. Here, we extend this discussion to the use of the CP* construction [134], a standard categorical construction yielding a theory CP*[**FHilb**] that contains both quantum and classical channels: i.e., we show that neither circuits interpreted in CP*[**FHilb**], nor simple constructions relying on CP*[**FHilb**], can adequately model superpositions of trajectories or causal decompositions. These considerations also apply to the use of the Karoubi envelope of CPM [**FHilb**], a category slightly larger than CP*[**FHilb**].

Let us first explain why it might be hoped that CP*[**FHilb**] would provide a sound basis for a representation of these scenarios.[3] The idea is that the objects of CP*[**FHilb**], being defined as C* algebras, can equivalently be thought of as arising from the choice of a preferred partition of a Hilbert space; therefore, the use of CP*[**FHilb**] would bypass the need for a definition of partitions 'by hand' as is done in the present thesis. From there, routes could be defined, not as a structure on maps, but rather as a purely diagrammatic piece of data, and it would suffice to impose that the interpretation of the diagrams in terms of morphisms in CP*[**FHilb**] be consistent with this diagrammatic information.

We will first explain why this strategy cannot in fact be implemented using CP*[**FHilb**]; then we will explain why we believe that the idea of defining routes as diagrammatic data to construct a suitable theory is at least as difficult as the approach taken in this thesis.

First, CP*[**FHilb**] is too restrictive to be used for the encoding of preferred partitions of Hilbert spaces. Indeed, if we define partitioned Hilbert spaces A^k and B^l as objects in CP*[**FHilb**], then the morphisms $A^k \to B^l$ in CP*[**FHilb**] can be defined as the CP linear maps from $\mathcal{L}(\mathcal{H}_A)$ to $\mathcal{L}(\mathcal{H}_B)$ that destroy coherence between the sectors of A and do not allow any coherence between those of B. However, we want the channels in our theory to possibly feature coherence between the sectors. This is in particular crucial in the examples of Sections 2.2 and 2.3: in superpositions of trajectories, the non-coherent case is a trivial and uninteresting one [49]; and in causal decompositions, all channels have to be unitary and thus perfectly coherent. CP*[**FHilb**] therefore cannot be used to model the structures we want to model.

We now comment on the more general idea of defining routes as mere diagrammatic data, rather than full-fledged morphisms, and simply asking for interpretations of diagrams to be consistent with that data. While this strategy has some advantages, it also presents significant drawbacks. First, it does not allow for the rewriting of a diagram in which, for instance, the composition of a box f and of a box g is replaced with a box $g \circ f$, as the 'route' diagrammatic data associated to this

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[3]We thank an anonymous QPL reviewer for raising this idea.

box will be undefined – unless compositions of routes are defined as well, which would bring one back towards a theory of routed maps as defined in this thesis.

Second, it makes the problem of defining physical maps more difficult. Indeed, to obtain such a definition, we have a crucial need for a notion of practical input and output spaces, one that can only be defined from the data given by the routes themselves.[4] Here again, in the absence of the structural handles provided by the acknowledgement that routes are not just graphical objects but morphisms with their own compositions, it would be difficult to express the conditions for the composition of such physical maps to be well-defined; expressing them would once again essentially amount to going back to a theory of routed maps.

A.3   Categorical perspective

A.3.1   Dagger symmetric monoidal categories

Let us introduce, in a non-technical way, the mathematical concepts which can be used to characterise the properties of the frameworks built in the present thesis. These concepts encapsulate the fact that a framework is suited for a diagrammatic representation of its maps in terms of circuits. The structure necessary for this mimics the basic structure of quantum theory: existence of sequential and parallel compositions, of identity maps, of trivial spaces, and of hermitian conjugates, all interacting in a natural way. Any theory with these features accepts sound and intuitive diagrammatic representations of its maps in terms of circuits [11, 60]. These concepts originate from *category theory*, a mathematical theory which has been at the centre of a recent re-formalisation of quantum theory [9, 11, 135, 136]. Our point here is not to present them in depth, but to provide the reader with an intuition of the simple structures that they express.

Categorical frameworks adopt the perspective of *process theories*: this means a theory is described not through its states, but through its *processes*, i.e. its dynamical transformations – states will be recovered as special cases of processes [11]. In the context of process theories, the main questions are about how processes can be composed together. A simple mathematical framework to describe sequential composition of processes is that of categories. A category contains two kinds of components: *objects*, corresponding to what would usually be called a space; and *morphisms* (or

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[4]The alternative would be to hardcode these 'practical input and output spaces' into objects, using, for instance, Karoubi envelopes. However, going this way would come at the cost of defining a very complex pseudo-tensor product structure. Indeed, one would for instance have to express the way in which L^k and R^k in (2.16) can be tensored in such a way as to yield not '$L^k \otimes R^{k'}$', but '$L^k \otimes R^{k'}$'; and more generally there should be pseudo-tensor products defined for every possible case of sectorial correlations. In the general case of non-sector-preserving routed maps, these tensor products would present very exotic features: for instance, the codomain of the pseudo-tensor product of two maps would in general depend on the routes they follow. Therefore 1) doing things in this way would still require to define routes as more than diagrammatic pieces of data, and 2) even though conceivable, it would require mathematical constructions which are more involved than those in this thesis. See also the discussion in Section 6.2.1.

maps), with a specified domain (i.e. input space) and a specified codomain (i.e. output space), both chosen among the objects of the category. Two morphisms can be sequentially composed if the codomain of the first matches the domain of the second: i.e. if $f : A \to B$ and $g : B \to C$ are maps, they can be composed to form a map $g \circ f : A \to C$. In a category, sequential composition is associative, and for any object A there exists an identity morphism $\mathrm{id}_A : A \to A$.

Some categories, called *symmetric monoidal categories* (SMC), also feature the structure for parallel composition of morphisms, in the form of an operation called the *tensor product*,[5] $\otimes$. The tensor product of two objects A and B yields an object $A \otimes B$, and the tensor product of two morphisms $f : A \to B$ and $g : C \to D$ yields a morphism $f \otimes g : A \otimes C \to B \otimes D$. The tensor product is associative. SMCs also feature a 'unit object' I satisfying $A \otimes I = I \otimes A = A$, which can be thought of as the trivial space of the theory; and swap morphisms, which are, for any pair of objects A and B, involutions from $A \otimes B$ to $B \otimes A$. These structures satisfy a set of various coherence conditions which ensure that they interplay appropriately (for instance, that sequential composition distributes over parallel composition, and so on). In an SMC, states on an object A are morphisms from the unit object I to A.

Finally, a dagger SMC is an SMC featuring an involution, called the adjoint, which, to any morphism $f : A \to B$, associates a morphism $f^\dagger : B \to A$. The adjoint satisfies various coherence conditions ensuring that it interplays consistently with the rest of the symmetric monoidal structure. Combinations of parallel and sequential compositions of maps in dagger SMCs can always be faithfully represented by so-called *circuit diagrams*, in which maps are represented by boxes, and objects are represented by wires. For instance, the theory of linear maps between finite-dimensional Hilbert spaces forms a dagger SMC **FHilb**. We refer the interested reader to Refs. [11, 137, 138] for accessible introductions to symmetric monoidal categories.

All the theories we will be considering in this thesis are dagger SMCs,[6] which makes them suitable for diagrammatic representation in terms of circuit diagrams [11, 60]. In the following appendices we shall give the main elements of the proofs that the theories discussed in this thesis form dagger SMCs; more refined proofs are available in Ref. [4].

A.3.2   Routed maps form a dagger SMC

In this appendix, we prove the following theorem, which can be thought of as a rigorous version of Theorem 3.1.1.

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[5]Note that what we call the 'tensor product' in this context is not necessarily the tensor product of linear maps.

[6]In fact, all the theories presented here are dagger compact categories: on top of the dagger symmetric monoidal structure, they feature some additional structure, which can be roughly described as corresponding to the existence of a Choi-Jamiołkowski isomorphism. In particular, this entails that they can be faithfully represented by *string diagrams*, an extension of circuit diagrams [11]. This is discussed in Ref. [4].

Theorem A.3.1. *Partitioned spaces and routed maps form, respectively, the objects and morphisms of a dagger SMC* **RoutedFHilb**, *in which:*

- *composition is given by pairwise composition;*

- *parallel composition is given on objects by $A^k \otimes B^l := (\mathcal{H}_A \otimes \mathcal{H}_B, \mathcal{Z}_A \times \mathcal{Z}_B, (\pi_A^k \otimes \mu_B^l)_{(k,l) \in \mathcal{Z}_A \times \mathcal{Z}_B})$, and on morphisms by the cartesian product on the routes together with the tensor product on the linear maps;*

- *the trivial space is the trivial partition of $\mathbb{C}$: $1_{\text{RoutedFHilb}} := (\mathbb{C}, \{*\}, (1))$;*

- *the adjoint of $(\lambda, f) : A^k \to B^l$ is $(\lambda, f)^\dagger := (\lambda^\top, f^\dagger) : B^l \to A^k$;*

We shall prove here the main features of **RoutedFHilb**'s dagger symmetric monoidal structure: that it is closed under sequential and parallel compositions and under taking adjoints, that sequential and parallel compositions are associative, and that parallel composition distributes over sequential composition. That the various coherence conditions are also satisfied can be proven easily. In the following we will freely use some partitioned Hilbert spaces $A^k = (\mathcal{H}_A, \mathcal{Z}_A, (\pi_A^k)_{k \in \mathcal{Z}_A})$, $B^l = (\mathcal{H}_B, \mathcal{Z}_B, (\mu_B^l)_{l \in \mathcal{Z}_B})$, $C^m = (\mathcal{H}_C, \mathcal{Z}_C, (\nu_C^m)_{m \in \mathcal{Z}_C})$, $D^n = (\mathcal{H}_D, \mathcal{Z}_D, (\eta_D^n)_{n \in \mathcal{Z}_D})$.

Let us first prove a useful equivalent definition of the fact that a linear map follows a route: a map $f : \mathcal{H}_A \to \mathcal{H}_B$ follows a route λ if and only if $\forall k, l, \lambda_k^l = 0 \implies \mu_B^l \circ f \circ \pi_A^k = 0$. Considering first the direct implication and supposing that f follows λ, one then has

$$
\begin{aligned}
0 &= f - f \\
&= \left(\sum_l \mu_B^l \right) \circ f \circ \left(\sum_k \pi_A^k \right) - \sum_{k,l} \lambda_k^l \cdot \mu_B^l \circ f \circ \pi_A^k \\
&= \sum_{k,l | \lambda_k^l = 0} \mu_B^l \circ f \circ \pi_A^k .
\end{aligned}
\tag{A.1}
$$

Hitting this equation with the μ^l's on the left and the π^k's on the left yields: $\forall k, l : \lambda_k^l = 0 \implies \mu_B^l \circ f \circ \pi_A^k = 0$. Reciprocally, supposing the latter, one has

$$
\begin{aligned}
f &= \left(\sum_l \mu_B^l \right) \circ f \circ \left(\sum_k \pi_A^k \right) \\
&= \sum_{k,l | \lambda_k^l = 1} \mu_B^l \circ f \circ \pi_A^k \\
&= \sum_{k,l} \lambda_k^l \cdot \mu_B^l \circ f \circ \pi_A^k .
\end{aligned}
\tag{A.2}
$$

We now prove that routed maps are closed under sequential composition. If we take two routed maps $(\lambda, f) : A^k \to B^l$ and $(\sigma, g) : B^l \to C^m$ and take indices k, m such that $(\sigma \circ \lambda)_k^m = \sum_l \sigma_l^m \lambda_k^l = 0$, we have $\nu_C^m \circ g \circ f \circ \pi_A^k = \nu_C^m \circ g \circ (\sum_l \mu_B^l) \circ f \circ \pi_A^k$.

Yet the fact that $\sum_l \sigma_l^m \lambda_k^l = 0$ implies that for any given l, one has either $\sigma_l^m = 0$ or $\lambda_k^l = 0$. The first case implies that $\nu_C^m \circ g \circ \mu_B^l = 0$, and the second that $\mu_B^l \circ f \circ \pi_A^k = 0$. Thus all the terms in this sum are null and $\nu_C^m \circ g \circ f \circ \pi_A^k = 0$, so $g \circ f$ follows $\sigma \circ \lambda$, so $(\sigma \circ \lambda, g \circ f)$ is a routed map.

For parallel composition, taking $(\lambda, f) : A^k \to C^m$ and $(\sigma, g) : B^l \to D^n$, we have that $(\lambda \times \sigma)_{kl}^{mn} = \lambda_k^m \sigma_l^n$. So $(\lambda \times \sigma)_{kl}^{mn} = 0$ implies that either λ_k^m or σ_l^n is null. In the first case, $\nu_C^m \circ f \circ \pi_A^k = 0$, in the second one, $\eta_D^n \circ g \circ \mu_B^l = 0$; so in both cases, $(\nu_C^m \otimes \eta_D^n) \circ (f \otimes g) \circ (\pi_A^k \otimes \mu_B^l) = (\nu_C^m \circ f \circ \pi_A^k) \otimes (\eta_D^n \circ g \circ \mu_B^l) = 0$. Therefore, $(\lambda \times \sigma, f \otimes g)$ is a routed map.

For closure under taking adjoints, take $(\lambda, f) : A^k \to B^l$. Then for given k and l, $(\lambda^\top)_l^k = 0 \implies \lambda_k^l = 0 \implies \mu_B^l \circ f \circ \pi_A^k = 0 \implies (\mu_B^l \circ f \circ \pi_A^k)^\dagger = 0 \implies \pi_A^k \circ f^\dagger \circ \mu_B^l = 0$, where in the last implication we used the fact that orthogonal projectors are self-adjoint. $(\lambda^\top, f^\dagger)$ is thus a routed map.

Finally, that parallel and sequential compositions are associative (both on objects and on morphisms) and that the former distributes over the latter is direct as these were defined pairwise from sequential and parallel compositions which possess all these properties.

A.3.3 Routed CPMs form a dagger SMC

Here, we prove the analogue of Theorem A.3.1 for the case of routed completely positive maps. Let us start with a formal characterisation of how an orthogonal partition of a Hilbert space $\mathcal{H}_A$ induces an orthogonal partition of the space $\mathcal{L}(\mathcal{H}_A)$ of linear operators on $\mathcal{H}_A$.

Theorem A.3.2. *If $(\pi_A^k)_{k \in \mathcal{Z}_A}$ is an orthogonal partition of $\mathcal{H}_A$, then, defining the following linear operators on $\mathcal{L}(\mathcal{H}_A)$,*

$$\forall k, k', \ \tilde{\pi}^{k,k'} : \rho \mapsto \pi_A^k \circ \rho \circ \pi_A^{k'}, \tag{A.3}$$

$(\tilde{\pi}^{k,k'})_{(k,k') \in \mathcal{Z}_A \times \mathcal{Z}_A}$ is an orthogonal partition of $\mathcal{L}(\mathcal{H}_A)$ (with respect to the Hilbert-Schmidt inner product).

The proof is direct.

We can then characterise the dagger SMC formed by routed CPMs.

Theorem A.3.3. *There exists a dagger SMC* **RoutedCPMFHilb***, in which:*

- *objects are partitioned Hilbert spaces $A^{kk'} := (\mathcal{L}(\mathcal{H}_A), \mathcal{Z}_A \times \mathcal{Z}_A, (\tilde{\pi}^{k,k'})_{(k,k') \in \mathcal{Z}_A \times \mathcal{Z}_A})$, whose underlying space is a space of linear operators on a given Hilbert space, and whose orthogonal partition is one obtained from an orthogonal partition of this Hilbert space through the procedure of Theorem A.3.2;*

- *morphisms $A^{kk'} \to B^{ll'}$ are routed maps $(\Lambda, \mathcal{C})$, with Λ a completely positive relation and $\mathcal{C}$ a completely positive linear map;*

- *composition is given by pairwise composition;*

- *parallel composition is given on objects by $A^{kk'} \otimes B^{ll'} := (\mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B), \mathcal{Z}_A \times \mathcal{Z}_B \times \mathcal{Z}_A \times \mathcal{Z}_B, (\tilde{\pi}_A^{k,k'} \otimes \tilde{\mu}_B^{l,l'})_{k,l,k',l'})$, and on morphisms by the cartesian product on the routes together with the tensor product on the linear maps;*

- *the trivial space is the trivial partition of $\mathcal{L}(\mathbb{C})$: $1_{\mathbf{RoutedCPMFHilb}} := (\mathcal{L}(\mathbb{C}), \{*\}, (1))$;*

- *the adjoint of $(\Lambda, \mathcal{C})$ is $(\Lambda, \mathcal{C})^\dagger := (\Lambda^\top, \mathcal{C}^\dagger)$.*

The proof is very similar to the proof of Theorem A.3.1. Closure under sequential and parallel composition come from the combination of two facts: that sequential and parallel compositions of routed maps are themselves routed maps, and that sequential and parallel compositions of completely positive linear maps and relations are themselves completely positive. The first fact was proven in Appendix A.3.2; the second comes from the fact that completely positive morphisms can be obtained from the universal construction of Selinger [105] for any †-compact category, and therefore form a †-compact category themselves. The same facts entail that routed completely positive maps are closed under taking adjoints. Finally, that parallel and sequential compositions are associative (both on objects and on morphisms) and that the former distributes over the latter is direct as these were defined pairwise from sequential and parallel compositions which possess all these properties.

A.4 Compositions of practical isometries

We first prove Theorem 3.1.2. Let $(\lambda, U) : A^k \to B^l$ and $(\sigma, V) : B^l \to C^m$ be practical isometries, such that λ and σ satisfy (3.6). Then the practical input set of $\sigma \circ \lambda$ is $\mathcal{S}_{\sigma \circ \lambda} = \lambda^\top[\mathcal{S}_\sigma] \subseteq \mathcal{S}_\lambda$. The practical input space of $(\sigma, V) \circ (\lambda, U)$ is therefore $\mathcal{H}_A^{\mathcal{S}_{\sigma \circ \lambda}} \subseteq \mathcal{H}_A^{\mathcal{S}_\lambda}$. As U is a partial isometry with initial subspace $\mathcal{H}_A^{\mathcal{S}_\lambda}$, it is in particular an isometry when restricted to $\mathcal{H}_A^{\mathcal{S}_{\sigma \circ \lambda}}$. Moreover, condition (3.6) and the fact that U follows λ imply that $U(\mathcal{H}_A^{\mathcal{S}_{\sigma \circ \lambda}}) = U(\mathcal{H}_A^{\lambda^\top[\mathcal{S}_\sigma]}) \subseteq \mathcal{H}_B^{(\lambda \circ \lambda^\top)[\mathcal{S}_\sigma]} \subseteq \mathcal{H}_B^{\mathcal{S}_\sigma}$. Therefore, as V is a partial isometry with initial subspace $\mathcal{H}_B^{\mathcal{S}_\sigma}$, it is in particular an isometry when restricted to $U(\mathcal{H}_A^{\mathcal{S}_{\sigma \circ \lambda}})$. It follows that $V \circ U$ is an isometry when restricted to $\mathcal{H}_A^{\mathcal{S}_{\sigma \circ \lambda}}$; so $(\sigma, V) \circ (\lambda, U)$ is a practical isometry.

We now prove that parallel composition of practical isometries always yields practical isometries. Let $(\lambda, U) : A^k \to B^l$ and $(\sigma, V) : C^m \to D^n$ be two practical isometries. Then $\mathcal{S}_{\lambda \times \sigma} = \mathcal{S}_\lambda \times \mathcal{S}_\sigma$, so $(\mathcal{H}_A \otimes \mathcal{H}_B)^{\mathcal{S}_{\lambda \times \sigma}} = \mathcal{H}_A^{\mathcal{S}_\lambda} \otimes \mathcal{H}_B^{\mathcal{S}_\sigma}$. The restriction of $U \otimes V$ to $(\mathcal{H}_A \otimes \mathcal{H}_B)^{\mathcal{S}_{\lambda \times \sigma}}$ is thus the tensor product of the restriction of U to $\mathcal{H}_A^{\mathcal{S}_\lambda}$ with the restriction of V to $\mathcal{H}_B^{\mathcal{S}_\sigma}$. As both of these are isometries, $(\lambda, U) \otimes (\sigma, V)$ is a practical isometry. The rest of the proof for the case of practical unitaries is similar.

A.5   Computing the accessible space

In this Appendix, we provide a more formal justification of the method presented in Section 3.2.3 to compute the accessible space corresponding to a slice in a given routed diagram.

Let us start with a formal definition of the accessible space. We take a routed circuit and pick a slice in it. We restrict ourselves to considering only the interpretation of this diagram in the theory of relations; considering the 'linear map' part of the interpretations is not important here, as we will only use the route information. We call $\mathcal{Z}$ the set of possible values of the indices in our slice, $\mathcal{P}$ the set of possible values of the indices of the open wires at the bottom of the diagram and $\mathcal{F}$ that of the open wires at the top of the diagram. We will consider what our diagram yields if we insert a given relation at this slice; given a relation $\lambda : \mathcal{Z} \to \mathcal{Z}$, we call $\mathcal{E}(\lambda) : \mathcal{P} \to \mathcal{F}$ the interpretation of the diagram when λ is inserted at the slice.

For any $k \in \mathcal{Z}$, let us define the relation $\varpi[k] : \mathcal{Z} \to \mathcal{Z}$ by $\varpi[k]_{k'}^{k''} = \delta_{kk'}^{kk''}$. We say that $k \in \mathcal{Z}^{\text{non-acc}}$ if $\mathcal{E}(\varpi[k]) = 0$, and define $\mathcal{Z}^{\text{acc}}$ as the complement of $\mathcal{Z}^{\text{non-acc}}$ in $\mathcal{Z}$. $\mathcal{Z}^{\text{acc}}$ corresponds to the index values that will form the accessible Hilbert space, i.e. we can define $\mathcal{H}^{\text{acc}} := \oplus_{k \in \mathcal{Z}^{\text{acc}}} \mathcal{H}^k$; indeed, the complementary set $\mathcal{Z}^{\text{non-acc}}$ is defined as containing those values of k which we know will be 'killed' by the routes.

Let us now introduce a useful lemma: if, for a finite set $\mathcal{Z}$, we note as $\varsigma : \{*\} \to \mathcal{Z}$ the 'full' relation defined by $\forall k \in \mathcal{Z}, \varsigma^k = 1$, then one has: $\forall \tau : \mathcal{P} \to \mathcal{F}, \tau = 0 \iff \varsigma_{\mathcal{F}}^{\top} \circ \tau \circ \varsigma_{\mathcal{P}} = 0$. The non trivial part here is the reverse implication; we can prove it by noting that the unique component of $\varsigma_{\mathcal{F}}^{\top} \circ \tau \circ \varsigma_{\mathcal{P}}$ is $\sum_{kk'} \tau_k^{k'}$; the rules of Boolean calculus therefore yield: $\varsigma_{\mathcal{F}}^{\top} \circ \tau \circ \varsigma_{\mathcal{P}} = 0 \implies \forall k, k', \tau_k^{k'} = 0 \implies \tau = 0$.

We thus have: $k \in \mathcal{Z}^{\text{acc}} \iff \varsigma_{\mathcal{F}}^{\top} \circ \mathcal{E}(\varpi[k]) \circ \varsigma_{\mathcal{P}} = 1$. One can see that the steps 1, 2, 3 and 4 in the procedure of Section 3.2.3 correspond to the computation of $\varsigma_{\mathcal{F}}^{\top} \circ \mathcal{E}(\varpi[k]) \circ \varsigma_{\mathcal{P}}$: in particular, the absence of summation on the indices of the slice corresponds to the insertion of $\varpi[k]$, and the summation over the indices of the input and output open wires corresponds to the composition with the ς's. Step 5 thus recovers our formal definition of the accessible space.

A.6   Sectorial constraints and Kraus representations

We first prove Theorem 3.3.3. We take a routed CPM $(\Lambda, \mathcal{C}) : A^{kk'} \to B^{ll'}$. One can prove, in a similar way to how it was done for linear maps in Appendix A.3.2, that condition (3.14) is equivalent to the fact that for all k, k', l, l', $\Lambda_{kk'}^{ll'} = 0 \implies \forall \rho, \mu_B^l \circ \mathcal{C}(\pi_A^k \circ \rho \circ \pi_A^{k'}) \circ \mu_B^{l'} = 0$. Let us take k, k', l, l' such that $\dot{\Lambda}_k^l = 0$, and a Kraus representation $\{K_i\}_i$ of $\mathcal{C}$. If we take any states $|\psi\rangle \in \mathcal{H}_A^k, |\phi\rangle \in \mathcal{H}_B^l$, we have $\forall i, \langle\phi| K_i |\psi\rangle \langle\psi| K_i^{\dagger} |\phi\rangle \in \mathbb{R}^+$ and $\sum_i \langle\phi| K_i |\psi\rangle \langle\psi| K_i^{\dagger} |\phi\rangle = \langle\phi| \mathcal{C}(|\psi\rangle \langle\psi|) |\phi\rangle = 0$, which implies $\forall i, \langle\phi| K_i |\psi\rangle \langle\psi| K_i^{\dagger} |\phi\rangle = 0$. As this is true for any $|\psi\rangle \in \mathcal{H}_A^k, |\phi\rangle \in \mathcal{H}_B^l$, one has $\forall i, \mu_B^l K_i \pi_A^k = 0$. Thus each of the K_i's follow $\dot{\Lambda}$.

Let us prove the reverse implication for a Λ with full coherence. If we take $\mathcal{C}$ with Kraus representation $\{K_i\}_i$ such that each of the K_i's follow $\dot{\Lambda}$, then for all k, k', l, l', $\Lambda^{ll'}_{kk'} = \dot{\Lambda}^l_k \dot{\Lambda}^{l'}_{k'} = 0$ implies that at least one of $\dot{\Lambda}^l_k$ and $\dot{\Lambda}^{l'}_{k'}$ is null, and thus that for any given i, at least one of $\mu^l_B K_i \pi^k_A$ and $\mu^{l'}_B K_i \pi^{k'}_A$ is null. Therefore $\forall \rho, \mu^l_B \circ \mathcal{C}(\pi^k_A \circ \rho \circ \pi^{k'}_A) \circ \mu^{l'}_B = \sum_i \mu^l_B K_i \pi^k_A \rho \pi^{k'}_A K^\dagger_i \mu^{l'}_B = 0$, so $\mathcal{C}$ follows Λ.

We turn to the proof of Theorem 3.3.4. Let us take a completely positive route Λ with full decoherence, i.e. $\Lambda^{ll'}_{kk'} = \dot{\Lambda}^l_k \delta_{kk'} \delta^{ll'}$, and a completely positive map $\mathcal{C}$ following Λ. Then $\forall \rho, \mathcal{C}(\rho) = \sum_{k,l} \dot{\Lambda}^l_k \mu^l_B \circ \mathcal{C}(\pi^k_A \circ \rho \circ \pi^k_A) \circ \mu^l_B$; thus if we define, for any k, l such that $\dot{\Lambda}^l_k = 1$, $\mathcal{C}^l_k : \rho \mapsto \mu^l_B \circ \mathcal{C}(\pi^k_A \circ \rho \circ \pi^k_A) \circ \mu^l_B$, one has $\mathcal{C} = \sum_{k,l | \dot{\Lambda}^l_k = 1} \mathcal{C}^l_k$, and each of the $\mathcal{C}^l_k$'s is a completely postive map from $\mathcal{L}(\mathcal{H}^k_A)$ to $\mathcal{L}(\mathcal{H}^l_B)$. Taking a Kraus representation for each of the $\mathcal{C}^l_k$'s yields a Kraus representation of $\mathcal{C}$ of the form given by Theorem 3.3.4. The reverse implication is direct.

A.7   A formal construction of index-matching routed maps

A.7.1   Index-matching routed maps as a category

In this appendix, we present a formal construction of the framework of index-matching routed maps, which was introduced in a more intuitive way in Section 3.4.

We first need to formally define *multiple indexings*: families of indices, each with its length, i.e. the number of different values it can take.

Definition A.7.1. *A (finite)* ***index family*** *is a finite set $\mathcal{X}$ equipped with a 'length' function $l : \mathcal{X} \to \mathbb{N}$. Given such an index family, the corresponding (finite)* ***multiple indexing*** *is the set $\bar{\mathcal{X}} := \bigtimes_{x \in \mathcal{X}} [\![1, l(x)]\!]$, where $\forall n, [\![1, n]\!] := \{m \in \mathbb{N} | 1 \leq m \leq n\}$ and $\bigtimes$ denotes the cartesian product.*

$\mathcal{X}$ serves as an 'indexing of indices': it gives names to the different possible indices.

Routes in index-matching routed maps have to be *corelations* [139] (this is written with a single r). Corelations will be used to define, among the union of their input and output indices, clusters of indices which will be matched (i.e. will 'be the same index').

Definition A.7.2. *Let $\mathcal{X}_A$ and $\mathcal{X}_B$ be two finite sets. A (finite)* ***corelation*** *$\kappa : \mathcal{X}_A \to \mathcal{X}_B$ is an equivalence relation on the disjoint union $\mathcal{X}_A \sqcup \mathcal{X}_B$.*

Finite corelations can be composed sequentially and in parallel, and form a dagger SMC **FCoRel** [140].

Definition A.7.3. *Let $\mathcal{X}_A$ and $\mathcal{X}_B$ be finite index families. An* ***index-matching*** *from $\mathcal{X}_A$ to $\mathcal{X}_B$ is a corelation $\kappa : \mathcal{X}_A \to \mathcal{X}_B$ such that: $\forall x, x' \in \mathcal{X}_A \sqcup \mathcal{X}_B, x \overset{\kappa}{\sim} x' \implies l(x) = l(x')$.*

It is easy to see that the theory in which objects are index families and morphisms are index-matchings itself forms a dagger SMC **FMatch**. The following ensures that index-matchings are just special cases of relations: for each index-matching between

index families, there is a corresponding relation between the corresponding multiple indexings, in a consistent way. This can be considered as a formal way of defining the relation corresponding to an index-matching as made of Kronecker deltas determined by this index-matching.

Definition A.7.4. *For any index-matching $\kappa : \mathcal{X}_A \to \mathcal{X}_B$, the relation associated to κ is $\bar{\kappa} : \bar{\mathcal{X}}_A \to \bar{\mathcal{X}}_B$, defined by the following condition: an element $\vec{k} = (k_x)_{x \in \mathcal{X}_A}$ of $\bar{\mathcal{X}}_A$ is <u>not</u> related by $\bar{\kappa}$ to an element $(k_x)_{x \in \mathcal{X}_B}$ of $\bar{\mathcal{X}}_B$ if and only if there exist $x, x' \in \mathcal{X}_A \sqcup \mathcal{X}_B$ such that $x \overset{\kappa}{\sim} x'$ and $k_x \neq k_{x'}$.*

Going from index families to multiple indexings, and from index-matchings to relations, is an operation which preserves the dagger SMC structure of **FMatch** into that of **FRel**.

Theorem A.7.1. *The 'bar' operation, which associates to an index family its corresponding multiple indexing, and to an index-matching its associated relation, is a functor of dagger SMCs.*

Proof. Let us first prove that it preserves sequential composition, i.e., $\overline{\kappa' \circ \kappa} = \bar{\kappa}' \circ \bar{\kappa}$. From $\overset{\kappa}{\sim}$ and $\overset{\kappa'}{\sim}$, one can form an equivalence relation $\sim$ on $\mathcal{X}_A \sqcup \mathcal{X}_B \sqcup \mathcal{X}_C$, of which $\overset{\kappa' \circ \kappa}{\sim}$ is the restriction to $\mathcal{X}_A \sqcup \mathcal{X}_C$. Suppose $(k_x)_{x \in \mathcal{X}_A} \overset{\overline{\kappa' \circ \kappa}}{\sim} (k_x)_{x \in \mathcal{X}_C}$; then $\forall x, x' \in \mathcal{X}_A \sqcup \mathcal{X}_C, x \overset{\kappa' \circ \kappa}{\sim} x' \implies k_x = k_{x'}$. One can thus complete this by finding a family $(k_x)_{x \in \mathcal{X}_B}$ such that: $\forall x, x' \in \mathcal{X}_A \sqcup \mathcal{X}_B \sqcup \mathcal{X}_C, x \sim x' \implies k_x = k_{x'}$. Then in particular $(k_x)_{x \in \mathcal{X}_A} \overset{\bar{\kappa}}{\sim} (k_x)_{x \in \mathcal{X}_B} \overset{\bar{\kappa}'}{\sim} (k_x)_{x \in \mathcal{X}_C}$, so $(k_x)_{x \in \mathcal{X}_A} \overset{\bar{\kappa}' \circ \bar{\kappa}}{\sim} (k_x)_{x \in \mathcal{X}_C}$.

Reciprocally, if $(k_x)_{x \in \mathcal{X}_A} \overset{\bar{\kappa}' \circ \bar{\kappa}}{\sim} (k_x)_{x \in \mathcal{X}_C}$; then there exists $(k_x)_{x \in \mathcal{X}_B}$ such that $(k_x)_{x \in \mathcal{X}_A} \overset{\bar{\kappa}}{\sim} (k_x)_{x \in \mathcal{X}_B} \overset{\bar{\kappa}'}{\sim} (k_x)_{x \in \mathcal{X}_C}$. If we take $x \in \mathcal{X}_A, x' \in \mathcal{X}_C$ such that $k_x \neq k_{x'}$, then for any $x'' \in \mathcal{X}_B$, at least one of the propositions $k_x = k_{x''}, k_{x''} = k_{x'}$ is false, so it is not possible that $x \overset{\kappa}{\sim} x'' \overset{\kappa'}{\sim} x'$, so $x \overset{\kappa' \circ \kappa}{\not\sim} x'$. With the same reasoning, one can prove the same thing if x and x' are both either in $\mathcal{X}_A$ or in $\mathcal{X}_C$ and $k_x \neq k_{x'}$. Thus $(k_x)_{x \in \mathcal{X}_A} \overset{\overline{\kappa' \circ \kappa}}{\sim} (k_x)_{x \in \mathcal{X}_C}$. From this implication and the previous one, it follows that $\overline{\kappa' \circ \kappa} = \bar{\kappa}' \circ \bar{\kappa}$.

It is then a routine check to prove that $\overline{\mathcal{X}_A \times \mathcal{X}_B} = \bar{\mathcal{X}}_A \times \bar{\mathcal{X}}_B$, $\overline{\kappa' \times \kappa} = \bar{\kappa}' \times \bar{\kappa}$, $\overline{\kappa^\top} = \bar{\kappa}^\top$, etc. $\qquad\square$

Thus, index-matchings can be seen as forming a subtheory of relations. This allows us to define notions for index-matchings from the notions for relations.

Definition A.7.5. *Let $(\mathcal{H}_A, \bar{\mathcal{X}}_A, (\pi^{\vec{k}})_{\vec{k} \in \bar{\mathcal{X}}_A})$ and $(\mathcal{H}_B, \bar{\mathcal{X}}_B, (\mu^{\vec{l}})_{\vec{l} \in \bar{\mathcal{X}}_B})$ be two partitioned spaces, where $\bar{\mathcal{X}}_A$ and $\bar{\mathcal{X}}_B$ are multiple indexings for index families $\mathcal{X}_A$ and $\mathcal{X}_B$, and let $\kappa : \mathcal{X}_A \to \mathcal{X}_B$ be an index-matching. A linear map $f : \mathcal{H}_A \to \mathcal{H}_B$ **follows the index-matching route** κ if it follows its associated relation $\bar{\kappa}$. The pair (κ, f) is then an **index-matching routed map**.*

The following is then direct.

Theorem A.7.2. *Index-matching routed maps form a dagger SMC **MatchedFHilb**, which is embedded into **RoutedFHilb**.*

A.7.2 Practical isometries and their composition

The definitions of practical isometries and practical unitaries in **RoutedFHilb** can be used in **MatchedFHilb** as well. In this context, Theorem 3.1.2 becomes more intuitive. First, we will define formally what it means to create and delete an index.

Definition A.7.6. *An index **created** (resp. **deleted**) by an index-matching κ is an equivalence class under κ which only contains output (resp. input) elements. Each of these elements is a **representative** of the created (resp. deleted) index.*

This leads to a characterisation of those compositions which do *not* satisfy Theorem 3.1.2.

Theorem A.7.3. *Let $\kappa : \mathcal{X}_A \to \mathcal{X}_B$ and $\iota : \mathcal{X}_B \to \mathcal{X}_C$ be index-matchings. The composition of κ and ι is improper for isometries if and only if there exists an index of length greater than or equal to 2 created by κ, such that, noting $\mathcal{W} \subseteq \mathcal{X}_B$ as the set of representatives of this index, ι matches at least one index in $\mathcal{W}$ with an index in $\mathcal{X}_B \setminus \mathcal{W}$.*

Proof. Let us note $\mathcal{X}_B \sqcup \mathcal{X}_B = \{(i,x) | i \in \{1,2\}, x \in \mathcal{X}_B\}$. It is easy to see that for $x \in \mathcal{X}_B$, $(1,x) \overset{\kappa \circ \kappa^\top}{\not\sim} (2,x)$ if and only if x's equivalence class under $\overset{\kappa}{\sim}$ is an index created by κ.

If the composition of κ and ι is not proper for isometries, there exist $\vec{k} \in \mathcal{S}_{\bar{\iota}}, \vec{k}' \in \bar{\mathcal{X}}_B \setminus \mathcal{S}_{\bar{\iota}}$ such that $\vec{k} \overset{\bar{\kappa} \circ \bar{\kappa}^\top}{\sim} \vec{k}'$. The fact that $\vec{k}' \in \bar{\mathcal{X}}_B \setminus \mathcal{S}_{\bar{\iota}}$ implies there exist $x, x' \in \mathcal{X}_B$ such that $x \overset{\iota}{\sim} x'$ and $k'_x \neq k'_{x'}$; the fact that $\vec{k} \in \mathcal{S}_{\bar{\iota}}$ implies that $k_x = k_{x'}$. That $(1,x) \overset{\kappa \circ \kappa^\top}{\sim} (2,x)$ and $(1,x') \overset{\kappa \circ \kappa^\top}{\sim} (2,x')$ would imply $k'_x = k_x = k_{x'} = k'_{x'}$, which would be a contradiction. Thus one of them (say, x) satisfies $(1,x) \overset{\kappa \circ \kappa^\top}{\not\sim} (2,x)$, so its equivalence class under $\overset{\kappa}{\sim}$ is an index created by κ. Calling this equivalence class $\mathcal{W} \subseteq \mathcal{X}_B$, one has $x' \in \mathcal{X}_B \setminus \mathcal{W}$, as $x' \in \mathcal{W}$ would imply $k'_x = k'_{x'}$. Finally, as $x \overset{\iota}{\sim} x'$, x and x' have the same length, and $k'_x \neq k'_{x'}$ implies that this length is at least 2; so the index which $\mathcal{W}$ represents has length at least 2.

Reciprocally, suppose there exists an index of length greater than or equal to 2 created by κ, with set of representatives $\mathcal{W} \subseteq \mathcal{X}_B$, such that ι matches $x \in \mathcal{W}$ with $x' \in \mathcal{X}_B \setminus \mathcal{W}$. Then there exists a $\vec{k}' \in \bar{\mathcal{X}}_B$ whose indices k'_y all have value 1, except for the y's in the equivalence class of x under $\overset{\kappa}{\sim}$, for which the value is $k'_y = 2$. We also define $\vec{k} \in \bar{\mathcal{X}}_B$ whose indices all have value 1. As the equivalence class of x under $\overset{\kappa}{\sim}$ is an index created by κ, $(1,x) \overset{\kappa \circ \kappa^\top}{\not\sim} (2,x)$, so $\vec{k} \overset{\bar{\kappa} \circ \bar{\kappa}^\top}{\sim} \vec{k}'$; yet $k \in \mathcal{S}_{\bar{\iota}}$ and $k' \notin \mathcal{S}_{\bar{\iota}}$, as $k'_x = 2 \neq k'_{x'} = 1$. Thus $\bar{\kappa} \circ \bar{\kappa}^\top (\mathcal{S}_{\bar{\iota}}) \not\subseteq \mathcal{S}_{\bar{\iota}}$ and the composition of $\bar{\kappa}$ and $\bar{\iota}$ is not suitable for isometries. $\square$

We now just need to spell out the corresponding requirement for unitaries.

Theorem A.7.4. *Let κ and ι be matchings of indices, with κ's codomain equal to ι's domain. The set of indices' names in the intermediary domain is noted $\mathcal{X}_B$. The composition of κ and ι is improper for unitaries if and only if at least one of the following is true:*

- *there exists an index of length greater than or equal to* 2 *created by κ such that, noting $\mathcal{W} \subseteq \mathcal{X}_B$ as the set of representatives of this index, ι matches at least one index in $\mathcal{W}$ with an index in $\mathcal{X}_B \setminus \mathcal{W}$;*

- *there exists an index of length greater than or equal to* 2 *deleted by ι such that, noting $\mathcal{W} \subseteq \mathcal{X}_B$ as the set of representatives of this index, κ matches at least one index in $\mathcal{W}$ with an index in $\mathcal{X}_B \setminus \mathcal{W}$.*

A.8 A formal construction of index-matching quantum circuits

A.8.1 Definition and composition

First, we define indexed wire systems.

Definition A.8.1. *An **indexed wire system** is a finite set I equipped with a set of indices K_I, a function $p_I : K_I \to I$ (indicating the indices' placement) and an equivalence relation $\sim_I$ on K_I.*

An indexed open directed acyclic graph (IODAG) will then be a map from one indexed wire system to another, taking the form of a multi-indexed directed acyclic graph.

Definition A.8.2. *Let I and O be two indexed wire systems. An **indexed open directed acyclic graph** $\Gamma : I \to O$ consists of the following:*

- *finite sets E_Γ (inner edges), N_Γ (nodes), and K_{E_Γ} (indices for the inner edges);*

- *a head function $h_\Gamma : I \sqcup E_\Gamma \to N_\Gamma$, a tail function $t_\Gamma : E_\Gamma \sqcup O \to N_\Gamma$, and a placing function $p_{E\Gamma} : K_{E_\Gamma} \to E_\Gamma$;*

- *an equivalence relation $\sim_\Gamma$ on $K_I \sqcup K_{E_\Gamma} \sqcup K_O$ which reduces to $\sim_I$ on K_I and to $\sim_O$ on K_O;*

such that the directed graph formed by the edges and nodes is acyclic.

Note that $h^{-1} : N_\Gamma \to \mathcal{P}(I \sqcup E_\Gamma)$ and $t^{-1} : N_\Gamma \to \mathcal{P}(E_\Gamma \sqcup O)$ both serve to specify, respectively, the subset of edges coming in a given node and the subset of edges going out of it. We will note $p_\Gamma := \langle p_I, p_{E\Gamma}, p_O \rangle$.

Most structural theorems for IODAGs will hold only up to isomorphism of IODAGs.

Definition A.8.3. *An **isomorphism of IODAGs** from Γ to Γ' is given by bijections $\alpha : E_\Gamma \to E'_{\Gamma'}$, $\beta : N_\Gamma \to N_{\Gamma'}$ and $\gamma : K_{E_\Gamma} \to K_{E_{\Gamma'}}$, such that $h_{\Gamma'} \circ \langle \mathrm{id}_I, \alpha \rangle = \beta \circ h_\Gamma$, $t_{\Gamma'} \circ \langle \alpha, \mathrm{id}_O \rangle = \beta \circ t_\Gamma$, $p_{E\Gamma'} \circ \alpha = \gamma \circ p_{E\Gamma}$, and such that $\langle \mathrm{id}_I, \alpha, \mathrm{id}_O \rangle$ maps $\sim_\Gamma$ to $\sim_{\Gamma'}$.*

We will therefore work with equivalence classes of IODAGs under isomorphisms of IODAGs. For the sake of clarity, we will still call such an equivalence class an IODAG, and usually refer to it by specifying a representative of this class.

We can then explain how to compose IODAGs. First, we will need a way to compose equivalence relations which, contrary to the standard composition of corelations, does not forget about the intermediary set.

Theorem A.8.1. *Let $\sim_1$ and $\sim_2$ be equivalence relations respectively defined on $A \sqcup B$ and $B \sqcup C$, and whose restrictions to B coincide. There exists a unique equivalence relation $\sim$ on $A \sqcup B \sqcup C$ such that $\sim$ reduces to $\sim_1$ on $A \sqcup B$, to $\sim_2$ on $B \sqcup C$, and to the composition of $\sim_1$ and $\sim_2$ (seen as corelations) on $A \sqcup C$. We will call $\sim$ the **non-forgetting composition** of $\sim_1$ and $\sim_2$.*

Proof. To build such an equivalence relation, let us take a cospan $A \xrightarrow{f_A} X \xleftarrow{f_B} B$ representing $\sim_1$, and a cospan $B \xrightarrow{g_B} Y \xleftarrow{g_C} C$ representing $\sim_2$. We can take the pushout of $X \xleftarrow{f_B} B \xrightarrow{g_B} Y$, given by $X \xrightarrow{i_1} Z \xleftarrow{i_2} Y$. This yields an arrow $\langle i_1 \circ f_A, i_1 \circ f_B, i_2 \circ g_C \rangle : A \sqcup B \sqcup C \to Z$, which defines an equivalence relation $\sim$ on $A \sqcup B \sqcup C$. As this is the standard way to define compositions of corelations, it follows that $\sim$ reduces to the composition of $\sim_1$ and $\sim_2$ (seen as corelations) on $A \sqcup C$.

Let us prove that $\sim$ reduces to $\sim_1$ on $A \sqcup B$ and to $\sim_2$ on $B \sqcup C$. The pushout Z is defined as the set of equivalence classes of $X \sqcup Y$ under the equivalence relation $\approx$ generated by the requirement: $x \approx y \iff \exists b, x = f_B(b) \wedge y = g_B(b)$. Yet, the fact that $\sim_1$ and $\sim_2$ coincide on B implies that there exists a partition $B = \amalg_i B_i$ and families $(x_i), (y_i)$ such that $\forall b \in B_i, f_B(b) = x_i \wedge g_B(b) = y_i$. Therefore, the equivalence classes of $\approx$ are the $\{x_i, y_i\}$ and the singletons $\{w\}$ where $w \notin f_B(B) \sqcup g_B(B)$. This implies that i_1 and i_2 are bijections. As a_1 is a bijection, two elements of $A \sqcup B$ are mapped to the same element of X if and only if they are mapped to the same element of Z; thus $\sim$ restricts to $\sim_1$ on $A \sqcup B$. Symmetrically, it restricts to $\sim_2$ on $B \sqcup C$.

Let us finally prove uniqueness; suppose that $\sim'$ satisfies the same requirements and that there exist d, d' such that $d \sim d'$ and $d \not\sim' d'$. Then, given that $\sim$ and $\sim'$ coincide on $A \sqcup B$ and on $B \sqcup C$, one must have $d \in A$ and $d' \in C$; this contradicts the fact that $\sim$ and $\sim'$ coincide on $A \sqcup C$. □

Definition A.8.4. *The sequential composition of two IODAGs $I \xrightarrow{\Gamma_1} J \xrightarrow{\Gamma_2} O$ is $\tilde{\Gamma} : I \to O$ defined by $\tilde{N} = N_1 \sqcup N_2$, $\tilde{E} = E_1 \sqcup J \sqcup E_2$, $\tilde{h} = \langle h_1, h_2 \rangle$, $\tilde{t} = \langle t_1, t_2 \rangle$, $K_{\tilde{E}} = K_{E_1} \sqcup K_J \sqcup K_{E_2}$, $\tilde{p}_{\tilde{E}} = \langle p_{E_1}, p_J, p_{E_2} \rangle$, and where $\sim_{\tilde{\Gamma}}$ is the non-forgetting composition of $\sim_1$ and $\sim_2$.*

Theorem A.8.2. *Sequential composition of IODAGs is associative.*

Proof. The only non-trivial thing to check is associativity of the non-forgetting composition. This is ensured by the way we built it using cospans and pushouts in the proof of Theorem A.8.1, and the fact that pushouts are unique up to isomorphism. □

Definition A.8.5. *Given two indexed wire systems I and I', their parallel composition is given by the set $I \sqcup I'$ and the structure $K_{I \sqcup I'} := K_I \sqcup K_{I'}$, $p_{I \sqcup I'} := \langle p_I, p_{I'} \rangle$ and $\sim_{I \sqcup I'} := \sim_I$*

$\sqcup \sim_{I'}$, *defined by the fact that it does not relate any elements of K_I and $K_{I'}$ and that it restricts to $\sim_I$ and $\sim_{I'}$ respectively on K_I and $K_{I'}$.*

Similarly, the parallel composition of $\Gamma : I \to O$ and $\Gamma' : I' \to O'$ is the IODAG $\Gamma \sqcup \Gamma' : I \sqcup I' \to O \sqcup O'$ given by taking disjoint unions on all of the relevant structure and defining the new equivalence relation in the same way.

The following is then direct.

Theorem A.8.3. *The parallel composition of IODAGs is associative, and distributes over sequential composition.*

Note, however, that the theory of IODAGs, thus defined, does not form a symmetric monoidal category, as it lacks identity morphisms. This can be dealt with by extending the definition of IODAGs, in order to allow *empty nodes*.

Definition A.8.6. *One can extend the definition of IODAGs by further equipping them with a set $\dot{N}_\Gamma \subseteq N_\Gamma$ of empty nodes, such that for a given $n \in \dot{N}_\Gamma$, n has only one ingoing wire $\mathrm{in}(n)$, and one outgoing wire $\mathrm{out}(n)$, whose indices are related in a consistent way: i.e. there exists a bijection $\xi_n^\Gamma : p_\Gamma^{-1}(\mathrm{in}(n)) \to p_\Gamma^{-1}(\mathrm{out}(n))$ such that $\forall k \in p_\Gamma^{-1}(\mathrm{in}(n)), k \sim_\Gamma \xi_n^\Gamma(k)$. One can further redefine a IODAG to be an equivalence class under the rewriting operations which consist in getting rid of some empty nodes and identifying their ingoing wire with their outgoing wire.*

Theorem A.8.4. *The theory of IODAGs with possibly empty nodes is a symmetric monoidal category.*

Proof. The non-trivial part is to prove that this theory has identity morphisms and swaps. The identity morphism from I to itself is given by the IODAG with no inner edges, $|I|$ empty nodes, each of which connects an element of I in the inputs with its counterpart in the outputs, and such that two elements $k, k' \in K_I \sqcup K_I$ are related if and only if they are related as elements of K_I. The swap from $I \sqcup J$ to $J \sqcup I$ is built in an analogous way. $\qquad \square$

We can now single out these IODAGs which are well indexed, for an interpretation in practical isometries and for one in practical unitaries.

Definition A.8.7. *Let $\Gamma : I \to O$ be a IODAG. For a given node n of Γ, the set of incoming indices for this node is $p_\Gamma^{-1} \circ h^{-1}(n)$, and the set of outgoing indices for this node is $p_\Gamma^{-1} \circ t^{-1}(n)$.*

*Let c be an equivalence class of $K_I \sqcup K_{E_\Gamma} \sqcup K_O$ under $\sim_\Gamma$, a **starting point** for c is a node n such that c has at least one representative in the set of outgoing indices of n, but no representatives in its incoming indices. An **endpoint** for c is defined symmetrically.*

*Γ is an **iso-IODAG** if each equivalence class c of $K_I \sqcup K_{E_\Gamma} \sqcup K_O$ under $\sim_\Gamma$ has at most one starting point, and has no starting point if it appears in the inputs of the diagram (i.e. if it has a representative in K_I).*

*Γ is a **uni-IODAG** if it is an iso-IODAG in which each equivalence class c of $K_I \sqcup K_{E_\Gamma} \sqcup K_O$ under $\sim_\Gamma$ has at most one endpoint, and has no endpoint if it appears in the outputs of the diagram (i.e. if it has a representative in K_O).*

Being well-indexed is a property preserved by composing diagrams, sequentially and in parallel:

Theorem A.8.5. *Sequential and parallel compositions of iso-IODAGs are iso-IODAGs, and sequential and parallel compositions of uni-IODAGs are uni-IODAGs.*

Proof. Let us take two iso-IODAGs $I \xrightarrow{\Gamma_1} J \xrightarrow{\Gamma_2} O$ and look at their sequential composition $\tilde{\Gamma}$. Take an equivalence class of indices c. Then the fact that $\sim_{\tilde{\Gamma}}$ reduces to $\sim_1$ on $K_I \sqcup K_J$ and to $\sim_2$ on $K_J \sqcup K_O$ implies that:

- if c has a representative in K_J, then there is an equivalence class c_1 under $\sim_1$ and an equivalence class c_2 under $\sim_2$ which correspond to c (i.e., an element belongs to one of these classes if and only if it belongs to c). As Γ_2 is an iso-IODAG and c_2 has a representative in K_J, it has no starting point in Γ_2, and thus neither does c. If c has a representative in K_I, then so does c_1, which therefore has no starting point in Γ_1; c then has no starting point in Γ. Otherwise, c_1 has one starting point, and thus so does c.

- if c has no representative in K_J, then its representatives are either all in Γ_1 or all in Γ_2; as both are iso-IODAGs, c therefore satisfies the conditions of Definition A.8.7.

$\tilde{\Gamma}$ is therefore an iso-IODAG. The rest of the proof for uni-IODAGs is symmetric.

For parallel compositions, as one has $\sim_{\Gamma_1 \sqcup \Gamma_2} = \sim_1 \sqcup \sim_2$, the set of representatives of a given class is included in one of the two diagrams; thus, that the requirements of Definition A.8.7 are satisfied by Γ_1 and by Γ_2 directly implies that they are satisfied by $\Gamma_1 \sqcup \Gamma_2$. $\qquad\square$

A.8.2 Interpretation

Finally, it is time to turn ourselves to interpretations of IODAGs in terms of index-matching routed maps. First, the index-matching routes are, in fact, defined even before having to interpret anything: they are given by the IODAGs alone.

Definition A.8.8. *Let Γ be an iso-IODAG. For each edge $e \in I \sqcup E_\Gamma \sqcup O$, we define its set of indices $\mathcal{X}_e := p_\Gamma^{-1}(e)$. For each node $n \in N_\Gamma$, we define its corelation $\kappa_n : \amalg_{e \in h^{-1}(n)} \mathcal{X}_e \to \amalg_{e' \in t^{-1}(n)} \mathcal{X}_{e'}$ by the fact that it relates two elements if and only if these are related under $\sim_\Gamma$. Furthermore, we define a pre-processing corelation κ_{pre} from K_I to itself by the requirement that it relates two elements of $K_I \sqcup K_I$ if and only if, when considered as elements of K_I, they are related by $\sim_I$.*

Before interpreting, we can show that the compositions of such corelations are suitable.

Lemma A.8.1. *Given an iso-IODAG (resp. a uni-IODAG) Γ, let us consider the corelation obtained by composing all of its nodes' corelations according to Γ's graph, then pre-composing the result with κ^{pre}. It is equal to κ_{tot}, the corelation which relates two elements*

of $K_I \sqcup K_O$ if and only if they are related by $\sim_\Gamma$. Furthermore, all the compositions in this construction are suitable for isometries (resp. for unitaries).

Proof. We call κ'_{tot} the corelation thus built; let us prove that it is equal to κ_{tot}. If we take two elements k, k' of K_I which are related by κ_{tot}, then they are related by κ_{pre} and therefore also by κ'_{tot}; the same holds if we take two elements of K_O which are related by κ_{tot}. If we take $k \in K_I$ and $k' \in K_O$ related by κ_{tot}, this means that they belong to a same equivalence class; as Γ is an iso-IODAG, this implies that this equivalence class has no starting point. There is therefore necessarily a path of related indices going downwards from k' to at least one index k'' in the inputs of the diagram, which implies that k' and k'' are related by κ'_{tot}. As k'' is itself related to k by κ_{pre} and therefore also by κ'_{tot}, transitivity allows us to conclude that k and k' are related by κ'_{tot}.

Reciprocally, if we take two elements of $K_I \sqcup K_O$ which are related by κ'_{tot}, this means that either they are related by κ_{pre}, or we can find a path of related indices connecting them through the graph of Γ. In the first case, they are clearly related by κ_{tot}; in the second case, as each of the index-matching route maps was obtained through a restriction of $\sim_\Gamma$, and as $\sim_\Gamma$ is transitive, this means that these two indices are also related by $\sim_\Gamma$, and therefore also by κ_{tot}.

Let us now prove, for the isometric case, that the compositions are suitable for isometries. One can build κ'_{tot} by foliating the graph, then composing the corelations layer by layer, starting with the pre-processing. The composition of the pre-processing with the first layer is suitable for isometries by Theorem A.7.3, as there are no indices created by the pre-processing. Say we have composed the pre-processing and the m first layers, yielding a corelation κ_m; its composition with layer $m + 1$ is suitable for isometries as well, again by Theorem A.7.3; indeed, an index created by κ_m is an index which is not present in the inputs of the diagram; it therefore has a starting point in the m first layers. This entails that the set of wires bearing this index is connected in the graph of Γ; therefore, all elements of the corresponding equivalence class in the outputs of the m first layers are related by κ_n. The $m + 1$ layer therefore cannot relate these elements with others, as it has to respect $\sim_\Gamma$. The rest of the proof in the unitary case is similar. $\square$

Definition A.8.9. *An **interpretation** of an iso-IODAG (resp. a uni-IODAG) $\Gamma : I \to O$ in practically isometric (resp. practically unitary) IMRMs consists of the following:*

- *a function* length $: K_I \sqcup K_{E_\Gamma} \sqcup K_O \to \mathbb{N}$, *satisfying* $k \sim_\Gamma k' \implies$ length$(k) =$ length(k');

- *a function* sys *which, to any $e \in I \sqcup E_\Gamma \sqcup O$, associates a partitioned Hilbert space of the form $(\mathcal{H}_A, \bar{X}_e, (\pi^{\vec{k}})_{\vec{k} \in \bar{X}_e})$, where $\bar{X}_e := \bigtimes_{x \in \mathcal{X}_e} [\![1, \text{length}(x)]\!]$;*

- *a function* morph *which, to any $n \in N_\Gamma$, associates a practically isometric (resp. practically unitary) index-matching routed map of the form (κ_n, f) from $\bigotimes_{e \in h^{-1}(n)} \text{sys}(e)$ to $\bigotimes_{e' \in t^{-1}(n)} \text{sys}(e')$.*

In addition, the input and output wires of an empty node must have the same interpretation and the interpretation of the empty node must be an identity morphism.

Interpreted IODAGs are called index-matching quantum circuits. The global index-matching routed map that an index-matching quantum circuit represents will be called its *meaning*.

Definition A.8.10. *Given an interpretation* $(\mathrm{length}, \mathrm{sys}, \mathrm{morph})$ *of an iso-IODAG, we define a pre-processing map* $(\kappa^{\mathrm{pre}}, \pi^{\mathrm{pre}})$ *from* $\bigotimes_{e \in I} \mathrm{sys}(e)$ *to itself, where* κ_{pre} *was defined in Definition A.8.8, and* $\pi^{\mathrm{pre}} := \sum_{\vec{k} \in \times_{e \in I} \bar{\mathcal{X}}_e} \bar{\kappa}_{\mathrm{pre}}^{\vec{k}, \vec{k}} \pi^{\vec{k}}$.

*The **meaning** of* $(\mathrm{length}, \mathrm{sys}, \mathrm{morph})$ *is then* $F \circ (\kappa_{\mathrm{pre}}, \pi^{\mathrm{pre}})$, *where F is the index-matching routed map obtained by composing the* $\mathrm{morph}(n)$ *according to the graph of Γ.*

Theorem A.8.6. *Given an interpretation of an iso-IODAG (resp. of a uni-IODAG) in practically isometric (resp. in practically unitary) IMRMs, its meaning is a practical isometry (resp. a practical unitary).*

Proof. This follows directly from Lemma A.8.1 and Theorems 3.1.2 and 3.1.3. □

Interpreting also plays well with sequential and parallel compositions.

Theorem A.8.7. *Let* $I \xrightarrow{\Gamma_1} J \xrightarrow{\Gamma_2} O$ *be two iso-IODAGs, whose sequential composition is noted* $\tilde{\Gamma}$, *and let* $(\mathrm{length}_1, \mathrm{sys}_1, \mathrm{morph}_1)$ *and* $(\mathrm{length}_2, \mathrm{sys}_2, \mathrm{morph}_2)$ *be respective interpretations which agree on J, i.e.* $\forall k \in K_J, \mathrm{length}_1(k) = \mathrm{length}_2(k)$ *and* $\forall e \in E_J, \mathrm{sys}_1(e) = \mathrm{sys}_2(e)$. *Then the sequential composition of their meanings is equal to the meaning of the interpretation of* $\tilde{\Gamma}$ *obtained by combining them.*

Proof. Let $\mathrm{mean}_1 = F_1 \circ (\kappa_1^{\mathrm{pre}}, \pi_1^{\mathrm{pre}})$ and $\mathrm{mean}_2 = F_2 \circ (\kappa_2^{\mathrm{pre}}, \pi_2^{\mathrm{pre}})$ be the respective meanings. By Lemma A.8.1, the index-matching route of mean_1 is κ_1^{tot}. In particular, for two elements of J related by $\sim_J$, they are related by κ_1^{tot}; therefore, $\mathrm{mean}_1 = (\kappa_2^{\mathrm{pre}}, \pi_2^{\mathrm{pre}}) \circ \mathrm{mean}_1$. This implies that $\mathrm{mean}_2 \circ \mathrm{mean}_1 = F_2 \circ F_1 \circ (\kappa_1^{\mathrm{pre}}, \pi_1^{\mathrm{pre}})$, which is the meaning of the corresponding interpretation of $\tilde{\Gamma}$. □

Theorem A.8.8. *Let Γ and Γ' be two iso-IODAGs, with respective interpretations* $(\mathrm{length}_1, \mathrm{sys}_1, \mathrm{morph}_1)$ *and* $(\mathrm{length}_2, \mathrm{sys}_2, \mathrm{morph}_2)$. *The parallel composition of their meanings is equal to the meaning of the interpretation* $(\langle \mathrm{length}_1, \mathrm{length}_2 \rangle, \langle \mathrm{sys}_1, \mathrm{sys}_2 \rangle, \langle \mathrm{morph}_1, \mathrm{morph}_2 \rangle)$ *of $\Gamma \sqcup \Gamma'$.*

Proof. Direct. □

Appendix B

Appendices for Chapter 4

B.1   A review of the terminology on coherent control in previous literature

The notion of 'coherent control' has been studied under several different names in the literature, which might lead to some confusion. In this appendix, we provide a review of the different terms previously used, arguing that they all essentially refer to the same notion. We will then motivate the choice of the term 'coherent control' employed in this thesis.

Coherent control was first considered for unitary gates in the work of Aharonov and coauthors [67]. In this work, controlled unitary gates were used to build what was called a 'superposition of time evolutions'. More precisely, the authors discussed the possibility of implementing evolutions of the form $\sum_j c_j U_j$, where the U_j's are unitary operators, and the c_j's are complex coefficients. It was proven that such an evolution could be realised, for arbitrary c_j's, using auxiliary systems and postselection. The protocol described in Ref. [67] consists in realising the controlled unitary gate $\sum_j |j\rangle\langle j| \otimes U_j$, initialising the control system in a superposition state, measuring the control system in a suitable basis, and then postselecting on a specific measurement outcome.

Another early instance was in the work of Åberg [57, 58], in which some of what would later come to be seen as the crucial features of coherent control were pointed out and analysed under different names. Indeed, Ref. [57] introduces the concept of so-called subspace-preserving channels, asking how their mathematical form can be obtained from that of their restrictions to each subspace, a procedure called *gluing of completely positive maps*, which is noted to be non-unique. This procedure is a mathematical avatar of the task of coherent control; and, even though the question of physical implementation is not discussed in detail, the comment on the non-uniqueness can be regarded as an early observation of the ill-definedness of the control between two quantum channels. This ill-definedness is noted to be due to the incompleteness of the description of the channels one wants to glue. An application of these methods to single-particle interferometry is described in Ref. [58].

Around the same time, Oi [68] studied the *interference of CP maps*, proposing that

the combination of quantum channels in an interferometic setup could reveal additional properties of their physical implementation that are not included in the mathematical expression of quantum channels. In the light of our results, the ability to probe additional properties of the implementation is due to the fact that the channels inserted in the interferometric setup are not the original channels, but rather sector-preserving channels of type $(1, d)$ which coincide with them on their d-dimensional sector. It is the properties of these sector-preserving channels, not of the original ones, that become visible through interferometry.

Finally, Chiribella and Kristjánsson [56] considered *superpositions of quantum channels*, in the context of a communication model where the information carriers move on a superpositions of trajectories. Even though this paper focused on applications to communication, its framework also yields an implementation of the task of coherent control, as shown by the present thesis. In this perspective, superpositions of trajectories represent one of the possible physical implementations of coherent control.

The term we adopted here, 'coherent control' (or sometimes 'quantum control', or simply 'control'), is commonly found in both experimental [14, 63, 119–121] and theoretical [13, 47, 64, 66, 96, 97, 111] works. Consistency with this relatively large body of works is one of the benefits of choosing the term 'control'. Moreover, this choice has the advantage of referring to a clearly defined operational task, rather than to analogies with properties of quantum states (such as 'superpositions of quantum evolutions' or 'superpositions of quantum channels'), to mathematical procedures ('gluing of CP maps'), to possible phenomena ('interference of CP maps'), or to specific types of physical implementations ('superpositions of trajectories').

B.2 Parametrising the coherent control between two channels

In this Appendix, we prove Theorem 4.2.2. We fix a Kraus representation $(A_i)_{i=1}^n$ of minimal length of $\mathcal{A}$. We first prove that any version of a controlled channel between $\mathcal{A}$ and $\mathcal{B}$ admits a Kraus decomposition $(K_j)_{j=1}^m$, where $m \geq n$, $K_j = \mathtt{ctrl}\text{-}(A_j, B_j)$ for $j \leq n$ and $K_j = \mathtt{ctrl}\text{-}(0, B_j)$ for $j > n$. Let us take such a channel, given by Kraus operators $(\mathtt{ctrl}\text{-}(A_i', B_i')_{i=1}^m$. The A_i' form a Kraus representation of $\mathcal{A}$; therefore, $m \geq n$ and there exists an unitary matrix $(V_{ji})_{i,j=1}^m$ such that $\sum_i V_{ji} A_i' = A_j$ for $j \leq n$ and 0 for $j > n$. Then, $(\sum_j V_{ji} K_i)_{j=1}^m$ is a Kraus representation of the right form for the controlled channel.

We now prove that, given two choices $(B_i)_{i=1}^m$ and $(B_j')_{j=1}^{m'}$ of Kraus representations for $\mathcal{B}$, the controlled channels that they define are equal if and only if $\forall i \leq n, B_i = B_i'$. First, suppose that the latter equation holds. Then, taking an isometry matrix $(V_{ji})_{n<i\leq m}^{n<j\leq m'}$ relating the Kraus decompositions $(B_i)_{i=n+1}^m$ and $(B_j)_{j=n+1}^{m'}$, we can complete it into a unitary matrix $(V_{ji})_{1\leq i\leq m}^{1\leq j\leq m'}$ by taking $\forall i, j \leq n, V_{ji} = \delta_{ji}$;

one then has $\forall i,j, \sum_i V_{ji}\texttt{ctrl-}(A_i, B_i) = \texttt{ctrl-}(A_j, B'_j)$. Reciprocally, suppose that the controlled channels defined by the choices $(B_i)_{i=1}^m$ and $(B'_j)_{j=1}^{m'}$ are equal. Taking then $(V_{ji})_{1 \leq i \leq m}^{1 \leq j \leq m'}$ to be an isometry matrix relating the associated Kraus decompositions, one has in particular $\forall i,j \leq n, \sum_i V_{ji}A_i = A_j$. Yet, that $(A_i)_{i=1}^n$ is a Kraus representation of minimal length implies in particular that the A_i's are linearly independent; therefore $\forall i,j \leq n, V_{ji} = \delta_{ji}$, which implies $\forall i \leq n, B'_i = B_i$.

B.3   Control of two noisy channels

In this Appendix, we propose a universal circuit implementation for all possible versions of the control between two noisy channels $\mathcal{A}$ and $\mathcal{B}$ from $\mathcal{L}(\mathcal{H}_{T_\text{in}})$ to $\mathcal{L}(\mathcal{H}_{T_\text{out}})$. To avoid clutter, we will take the isomorphisms $T_\text{in} \simeq S_\text{in}^1$ and $T_\text{out} \simeq S_\text{out}^1$ to be strict, that is, as will assume $T_\text{in} = S_\text{in}^1$ and $T_\text{out} = S_\text{out}^1$.

Recall that, as proven in Section 4.5, in the case where $\mathcal{A}$ and $\mathcal{B}$ are isometric channels the controlled version could be implemented using as resources sector-preserving channels from $\mathcal{L}(\mathcal{H}_{S_\text{in}}^0 \oplus \mathcal{H}_{S_\text{in}}^1)$ to $\mathcal{L}(\mathcal{H}_{S_\text{out}}^0 \oplus \mathcal{H}_{S_\text{out}}^1)$, where $\mathcal{H}_{S_\text{out}}^1 := \mathcal{H}_{S_\text{out}}$, $\mathcal{H}_{S_\text{in}}^1 := \mathcal{H}_{S_\text{in}}$, and $\mathcal{H}_{S_\text{in}}^0 \cong \mathcal{H}_{S_\text{out}}^0 \cong \mathbb{C}$, with these channels restricting respectively to $\mathcal{A}$ and $\mathcal{B}$ on $\mathcal{L}(\mathcal{H}_{S_\text{in}}^1)$. However, the controlled channels yielded by this method can feature full coherence only between at most one Kraus operator of $\mathcal{A}$ and one operator of $\mathcal{B}$.

Here, we shall therefore make use of more complex resources. These resources will be sector-preserving channels whose multi-dimensional output sector will not be $\mathcal{H}_{S_\text{out}}^1$, but $\mathcal{H}_{S_\text{out}}^1 \otimes \mathcal{H}_E^1$, where $\mathcal{H}_E^1$ is an auxiliary Hilbert space. The restrictions of these channels to this sector will have to yield $\mathcal{A}$ and $\mathcal{B}$ when E^1 is traced out. In other words, to get the full scope of controls between $\mathcal{A}$ and $\mathcal{B}$ we need to use sector-preserving channels that restrict to (possibly partial) purifications of $\mathcal{A}$ and $\mathcal{B}$ on their multi-dimensional sectors. Using such resources, the number of Kraus operators of $\mathcal{A}$ and $\mathcal{B}$ between which there can be full coherence in the controlled channel is capped by the dimension of $\mathcal{H}_E^1$. In particular a sufficiently large $\mathcal{H}_E^1$ will ensure that all possible controlled channels can be generated.

More formally, we define the superchannel 2-CTRL(E) from the superchannel 2-CTRL in the following way:[1]

---

[1]Here, we defined this superchannel as a routed one (also using the convention of contracting Kronecker deltas) for clarity, but this could also be arbitrarily expanded into a superchannel acting on all channels from $\mathcal{L}(\mathcal{H}_{S_\text{in}})$ to $\mathcal{L}(\oplus_{k \in \{0,1\}} \mathcal{H}_{S_\text{out}}^k \otimes \mathcal{H}_E^k)$. Note that when writing such a non-routed superchannel, one would have to write the combination of S_out and E as a single wire, as the way in which they combine to form $S_\text{out}^k E^k$ is not a tensor product and cannot be expressed using standard quantum circuits.

$$\text{2-CTRL}(E) := \text{2-CTRL} \quad . \tag{B.1}$$

Let us now prove that, for a given choice of E, 2-CTRL(E) can produce all controlled channels in which the number of coherent pairs of Kraus operators is less than the dimension of E.

Theorem B.3.1. *We fix an environment E with dimension D, and use the one-to-one parametrisation of the control between two channels provided by Theorem 4.2.2: i.e., given a Kraus representation $(A_i)_{i=1}^n$ of $\mathcal{A}$ of minimal length, the parametrisation is given by the choice of n Kraus operators B_i of $\mathcal{B}$.*

Then any choice of a control in which only the D first operators B_i are non-zero can be obtained from the use of the 2-CTRL(E) superchannel.

Proof. In the case $D = 1$ (i.e. that of the 2-CTRL superchannel), it can easily be computed, from the formula of Fig. 4.2, that any controlled version in which there is coherence between A_1 and B_1 can be obtained by plugging the channels $\widetilde{\mathcal{A}}^{A_1}$ and $\widetilde{\mathcal{B}}^{B_1}$ in 2-CTRL.

Considering now the case $D > 1$, let us take a version $\mathcal{C}$ of a control between $\mathcal{A}$ and $\mathcal{B}$ for which a Kraus representation is $\Big(|0\rangle\langle 0|_C \otimes A_1 + |1\rangle\langle 1|_C \otimes B_1, \ldots, |0\rangle\langle 0|_C \otimes A_D + |1\rangle\langle 1|_C \otimes B_D, |0\rangle\langle 0|_C \otimes A_{D+1}, \ldots, |0\rangle\langle 0|_C \otimes A_n, |1\rangle\langle 1|_C \otimes B_{D+1}, \ldots, |1\rangle\langle 1|_C \otimes B_m \Big)$. Then a (possibly partial) purification of $\mathcal{C}$ is given by the channel of type $CS_{\text{in}}^1 \to CS_{\text{out}}^1 E$ for which a Kraus representation is $\Big(\sum_{i=1}^D \big(|0\rangle\langle 0|_C \otimes A_i + |1\rangle\langle 1|_C \otimes B_i \big) \otimes |i\rangle_E, |0\rangle\langle 0|_C \otimes A_{D+1} \otimes |1\rangle_E, \ldots, |0\rangle\langle 0|_C \otimes A_n \otimes |1\rangle_E, |1\rangle\langle 1|_C \otimes B_{D+1} \otimes |1\rangle_E, \ldots, |1\rangle\langle 1|_C \otimes B_m \otimes |1\rangle_E \Big)$. This latter channel can be seen as being a version of a control between two channels $S_{\text{in}}^1 \to S_{\text{out}}^1 E^1$ with coherence between one pair of Kraus operators. By the first part of the proof, it can thus be obtained by applying the 2-CTRL superchannel to suitable sector-preserving channels of type $S_{\text{in}}^k \to S_{\text{out}}^k E^k$. Discarding E^1 then yields $\mathcal{C}$. The 2-CTRL(E) as defined in (B.1) thus yields $\mathcal{C}$ when applied to the same sector-preserving channels. $\square$

In particular, as any channel $S_{\text{in}}^1 \to S_{\text{out}}^1$ admits a Kraus representation of length less than the product of the dimensions of S_{in}^1 and S_{out}^1, all versions of controlled channels can be obtained from the use of the superchannel 2-CTRL(E) when E is of that dimension.

Appendix C

Appendices for Chapter 5

C.1 The relationship between the supermap and process matrix representations

Two equivalent but distinct mathematical frameworks are in use in the indefinite causal order literature to represent higher-order processes, stemming from two independent lines of work: one is that of supermaps [15, 17] (also called superchannels), and the other is that of process matrices [18, 59] (also called W-matrices). This can lead to some confusion. In this Appendix, we spell out the equivalence between the two pictures, in order to help readers more accustomed to the process matrix picture to translate our results and concepts from the supermap picture, that we use in this thesis.

In broad terms, supermaps and process matrices are equivalent mathematical representations of a same higher-order process, connected by the Choi-Jamiołkowski (CJ) isomorphism. What can add to the confusion is also that they stem from different conceptual points of view on the situations being modelled, and that the equivalence between these points of view might not be obvious at first sight. We will thus start with a conceptual discussion, before spelling out the mathematical equivalence. We will then further comment on how super*unitaries*, which are the focus of this thesis, can be translated to super*channels*: the jump is simply the standard one between the linear representation of pure quantum theory and the completely positive representation of mixed quantum theory.

C.1.1 At the conceptual level

The point of superchannels is to model higher-order transformations, mapping channels to channels, in the same way that channels map states to states. More precisely, in analogy with the fact that channels can be characterised as the only linear mappings $\mathcal{C} \in \text{Lin}\left[\text{Lin}(\mathcal{H}_A^{\text{in}}) \to \text{Lin}(\mathcal{H}_A^{\text{out}})\right]$ that preserve all quantum states – including quantum states on an extended system $\rho \in \text{Lin}[\mathcal{H}_A^{\text{in}} \otimes \mathcal{H}_X]$ –, superchannels are characterised [15] as the linear mappings

$$\mathcal{S} \in \text{Lin}\left[\text{Lin}\left[\text{Lin}(\mathcal{H}_A^{\text{in}}) \to \text{Lin}(\mathcal{H}_A^{\text{out}})\right] \to \text{Lin}\left[\text{Lin}(\mathcal{H}_P) \to \text{Lin}(\mathcal{H}_F)\right]\right] \qquad \text{(C.1)}$$

that preserve all quantum channels – including quantum channels on an extended system $\mathcal{C} \in \text{Lin}\left[\text{Lin}(\mathcal{H}_A^{\text{in}} \otimes \mathcal{H}_X) \to \text{Lin}(\mathcal{H}_A^{\text{out}} \otimes \mathcal{H}_Y)\right]$. Moreover, *multipartite* superchannels [16, 17] can act on pairs, or generally tuples, of channels, mapping them to one 'global' channel.[1] The conceptual idea is thus to combine 'Alice's channel' and 'Bob's channel' into a larger channel; it stems from an emphasis on a *computational* picture, focused on the study of architectures for quantum computation.

Another line of research, developed independently, adopts an *operational* picture, insisting instead on the idea of local agents performing quantum measurements – and crucially, getting classical outcomes [18]. Therefore, rather than on a notion of combining operations, it focuses on the task of computing joint probability distributions for these local outcomes. This is where process matrices come in naturally: taking $\mathcal{M}_i \in \text{Lin}[\text{Lin}[\mathcal{H}_A^{\text{in}}] \to \text{Lin}[\mathcal{H}_A^{\text{out}}]]$ as the CP map corresponding to Alice obtaining outcome i, and $M_i \in \text{Lin}[\mathcal{H}_A^{\text{in}} \otimes \mathcal{H}_A^{\text{out}}]$ as its CJ representation (see below for its mathematical definition) – and similarly taking N_j for Bob obtaining the outcome j –, one can write the joint probability compactly as

$$\mathcal{P}(i,j) = \text{Tr}\left[(M_i^T \otimes N_j^T) \circ W\right], \tag{C.2}$$

where $W \in \text{Lin}[\mathcal{H}_A^{\text{in}} \otimes \mathcal{H}_A^{\text{out}} \otimes \mathcal{H}_B^{\text{in}} \otimes \mathcal{H}_B^{\text{out}}]$ is the *process matrix*, which one asks to yield well-defined probabilities, through (C.2), for any choice of measurements on Alice and Bob's parts.

In order to allow for a notion of purification, the process matrix formalism was then extended [59] to model general higher-order operations, with W now also acting on a global past P and a global future F, and the RHS of (C.2) being taken to be a partial trace on all other systems, so that the LHS yields (the CJ representation of) a quantum operation $P \to F$. One can now see how this gets us closer, at least conceptually, to the notion of a superchannel. The original process matrices as defined in [18] can then be understood as akin to superchannels with a trivial output.

One might, however, worry that this overlooks the key conceptual difference: that process matrices relate not only channels, but also the probabilities of measurement outcomes. Shouldn't that be more general than superchannels? The key idea to understand why this worry is, in fact, unwarranted, is the fact that the obtaining of any measurement outcome can equivalently be modelled as the implementation of a deterministic channel acting on the system at hand and on an ancilla, together with a measurement outcome having been obtained by subsequently measuring the ancilla. In this way, one can recover the probabilities for measurements in the superchannel picture as well.

Before we turn to the mathematical equivalence, let us briefly comment on the respective strengths and weaknesses of the two representations. The main advantage

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[1]More precisely, bipartite superchannels were originally defined as acting on the larger space of all non-signalling channels on the tensor product of their two slots. However, it was proven at the same time that the well-defined superchannels on pairs of channels are exactly the same ones as superchannels on non-signalling channels, so we can overlook this difference.

of process matrices is the ability, in an operational picture, to compute joint probabilities in a straightforward and compact way, via the Hilbert-Schmidt inner product of (C.2). However, this strength becomes a weakness once one is interested in higher-order processes with a non-trivial output: because the process matrix is then a 'flattened' CJ representation of the process – i.e., an operator acting indistinctly on all the input and output Hilbert spaces involved, e.g. on $A^{\text{in}} \otimes A^{\text{out}} \otimes B^{\text{in}} \otimes B^{\text{out}} \otimes P \otimes F$ –, it smears out the distinction i) between the inputs and outputs of local operations (e.g. between A^{in} and A^{out}), and ii) between the inputs and the output of the higher-order transformation (e.g. between A^{in} and A^{out}, which correspond to one of the input channels, and P and F, which correspond to the output channel).

This flattening is the reason why the connectivity of a higher-order process is particularly difficult to parse in a process matrix: identities between systems, for instance, have to be represented not by identity operators but by maximally entangled states. Similarly, the tracing-out move of (C.2) lends itself badly to intuition and generally messes up the input/output structure. By contrast, the superchannel's type, as a map $\text{Chan}(A^{\text{in}} \to A^{\text{out}}) \times \text{Chan}(B^{\text{in}} \to B^{\text{out}}) \to \text{Chan}(P \to F)$, neatly encodes the different roles of the different spaces, and facilitates intuitions about the connectivity. In particular, as we are especially interested in a faithful and direct representation of the connectivity of processes, we found the superchannel picture more practical for the needs of the present thesis.

C.1.2 At the mathematical level

The process matrix picture relies on the Choi-Jamiolkowski (CJ) representation of CP maps [61, 62], which can be defined as follows. Consider a CP map $\mathcal{M}_A : A^{\text{in}} \to A^{\text{out}}$. We make a copy of the input system A^{in}, and consider the (unnormalised) maximally entangled state $|\Phi^+\rangle = \sum_i |ii\rangle$ on $A^{\text{in}} \otimes A^{\text{in}}$. The CJ representation M_A of $\mathcal{M}_A$ is then the positive operator on $A^{\text{in}} \otimes A^{\text{out}}$ obtained by feeding one half of this entangled state into $\mathcal{M}$:

$$M_A := (\mathcal{I} \otimes \mathcal{M}_A) |\Phi^+\rangle \langle \Phi^+| . \tag{C.3}$$

Process matrices were originally defined as operators mapping CJ representations of CP maps to probabilities via (C.2). In the bipartite case, they were therefore required to satisfy:

$$W \in \text{Lin}[\mathcal{H}_A^{\text{in}} \otimes \mathcal{H}_A^{\text{out}} \otimes \mathcal{H}_B^{\text{in}} \otimes \mathcal{H}_B^{\text{out}}] ,$$
$$W \geq 0 , \tag{C.4}$$
$$\text{Tr}\left[(M^T \otimes N^T) \circ W \right] = 1 \quad \forall M \, \forall N ,$$

where M and N can be CJ matrices for any pair of *channels* for Alice and Bob. The positivity requirement buys us positive probabilities; the last requirement ensures that our probability distributions are normalised.

In Ref. [59], the definition of process matrices was extended so that they output a CJ matrix for a CP map from a 'past' system P to a 'future' system F. In the bipartite case, the extended process matrix $W \in \mathrm{Lin}[\mathcal{H}_P \otimes \mathcal{H}_A^{\mathrm{in}} \otimes \mathcal{H}_A^{\mathrm{out}} \otimes \mathcal{H}_B^{\mathrm{in}} \otimes \mathcal{H}_B^{\mathrm{out}} \otimes \mathcal{H}_F]$ maps CJ matrices M and N to a CJ matrix $G := \mathrm{Tr}_{A^{\mathrm{in}} A^{\mathrm{out}} B^{\mathrm{in}} B^{\mathrm{out}}} \left[(M^T \otimes N^T) \circ W \right] \in \mathrm{Lin}[\mathcal{H}_P \otimes \mathcal{H}_F]$. Now, rather than requiring that we map CP maps to positive and normalised probabilities, we need to require that we map CP maps to CP maps, and channels to channels. This is guaranteed by the following conditions:

$$W \in \mathrm{Lin}[\mathcal{H}_P \otimes \mathcal{H}_A^{\mathrm{in}} \otimes \mathcal{H}_A^{\mathrm{out}} \otimes \mathcal{H}_B^{\mathrm{in}} \otimes \mathcal{H}_B^{\mathrm{out}} \otimes \mathcal{H}_F],$$
$$W \geq 0, \tag{C.5}$$
$$\mathrm{Tr}_{A^{\mathrm{in}} A^{\mathrm{out}} B^{\mathrm{in}} B^{\mathrm{out}}} \left[(M^T \otimes N^T) \circ W \right] = G \quad \forall M \; \forall N,$$

where M and N represent any channels for Alice and Bob, and we require that G represents a channel from P to F. The definitions for the original and the extended process matrices generalise in an obvious way to the multipartite case.

The original process matrices are special cases of these more general process matrices, in which the global 'past' and 'future' systems P and F are one-dimensional, since in this case probabilities are CP maps and the number 1 is a channel. On the other hand, when one considers any particular state-preparation at P, and traces out F, any of these new, extended process matrices gives rise to a process matrix as originally defined in (C.4)[84].

We now demonstrate the equivalence of the extended process matrices and superchannels. More precisely, we show that every extended process matrix uniquely defines a valid superchannel, and vice versa. A bipartite process matrix W defines a superchannel $\mathcal{S}$ in the following way:

$$\mathcal{S}(\mathcal{M}, \mathcal{N}) := \mathrm{Choi}^{-1} \left(\mathrm{Tr}_{A^{\mathrm{in}} A^{\mathrm{out}} B^{\mathrm{in}} B^{\mathrm{out}}} \left[(M^T \otimes N^T) \circ W \right] \right), \tag{C.6}$$

where $\mathcal{M} : \tilde{A}^{\mathrm{in}} \otimes A^{\mathrm{in}} \to \tilde{A}^{\mathrm{out}} \otimes A^{\mathrm{out}}$ is Alice's channel, which also acts on ancillas, and M is its CJ representation, and similarly for $\mathcal{N}$ and N.

One might initially worry that $\mathcal{S}$ need not always be a superchannel, since the extended process matrices were only defined with respect to input CP maps without ancillas, but a superchannel must also preserve channels with ancillas. However, the positivity of W ensures that $G \geq 0$ where

$$\begin{aligned} G : &= \mathrm{Tr}_{A^{\mathrm{in}} A^{\mathrm{out}} B^{\mathrm{in}} B^{\mathrm{out}}} \left[(M^T \otimes N^T) \circ W \right] \\ &\in \mathrm{Lin}[\mathcal{H}_P \otimes \mathcal{H}_{\tilde{A}}^{\mathrm{in}} \otimes \mathcal{H}_{\tilde{B}}^{\mathrm{in}} \otimes \mathcal{H}_F \otimes \mathcal{H}_{\tilde{A}}^{\mathrm{out}} \otimes \mathcal{H}_{\tilde{B}}^{\mathrm{out}}]. \end{aligned} \tag{C.7}$$

A positive CJ matrix always represents a CP map, meaning that $\mathrm{Choi}^{-1}(G)$ is indeed a CP map from the past and ancillary inputs, to the future and ancillary outputs. Then the last condition in (C.5) ensures that $\mathcal{S}$ maps channels with ancillas to other channels, meaning that $\mathcal{S}$ is indeed a superchannel.

To see how a bipartite superchannel $\mathcal{S}$ defines a process matrix W, we suppose that Alice and Bob both insert swap channels into the superchannel. The process matrix is then the CJ representation of the resulting channel:

$$W := \mathrm{Choi}\left(\mathcal{S}(\texttt{SWAP}, \texttt{SWAP})\right). \tag{C.8}$$

The positivity of W follows from the complete positivity of the channel $\mathcal{S}(\texttt{SWAP}, \texttt{SWAP})$. One can show that the mapping on (CJ representations of) channels provided by W is the same as the mapping provided by $\mathcal{S}$

$$\mathrm{Tr}_{A^{\mathrm{in}} A^{\mathrm{out}} B^{\mathrm{in}} B^{\mathrm{out}}} \left[(M^T \otimes N^T) \circ W \right] = G = \mathrm{Choi}(\mathcal{S}(\mathcal{M}, \mathcal{N})), \tag{C.9}$$

meaning the last requirement of (C.5) will also be satisfied.

Rather than superchannels, this work concentrates on what we call *superunitaries* – that is, linear mappings from a set of unitary operators to another unitary operator. To connect these to process matrices, we note that every superunitary uniquely defines a 'unitary superchannel' – that is, a superchannel that always returns a unitary channel when you feed it a set of unitary channels. Given a superunitary S, we define a unitary superchannel in an obvious way:

$$\mathcal{S}(\mathcal{U}, \mathcal{V}) := [S(U, V)] \, (\cdot) \, [S(U, V)]^\dagger \, ; \tag{C.10}$$

that is, the action of $\mathcal{S}$ on the channels $\mathcal{U} := U(\cdot)U^\dagger$ and $\mathcal{V} := V(\cdot)V^\dagger$ is just the channel corresponding to the action of S on U and V. The action of this superchannel on more general channels can then be calculated using the Stinespring dilation. Conversely, any unitary superchannel defines a superunitary, up to an irrelevant global phase.

We have shown that i) superchannels are equivalent to process matrices and ii) superunitaries are equivalent to unitary superchannels (up to phase). Now it follows trivially that superunitaries are equivalent to unitary process matrices – that is, the process matrices that map unitary channels (possibly with ancillas) to unitary channels. As proven in Ref. [59], these are precisely the process matrices that can be written in the form $W = |U_w\rangle \langle U_w|$ where

$$|U_w\rangle := (I \otimes U_w) |\Phi^+\rangle \tag{C.11}$$

is a CJ *vector* representing a unitary operator U_w.

C.2   Technical definitions and proofs

C.2.1   Notations

In this appendix, we spell out our framework in fully technical terms, and prove its central theorem, ensuring that the routed graphs that satisfy the two principles define routed superunitaries.

To do this, and in particular to prove the theorem, we will have to deal with complicated operators, often acting on arbitrary numbers of factored spaces. We therefore introduced some notational techniques to avoid unnecessary clutter, which we will present and motivate here.

The first of these techniques is *padding*. The idea is to have operators act on spaces larger than the ones they were originally defined to act on, simply by tensoring them with identity operators. For instance, we can have $f \in \mathcal{L}(\mathcal{H}_A)$ act on $\mathcal{H}_A \otimes \mathcal{H}_B$, by considering $f \otimes I_B$. However, when – as will often be the case in what follows – there is an arbitrarily large number of factors, and f formally only acts on an arbitrary subset of them, it becomes very heavy notationally, and of limited mathematical interest, to keep track explicitly of which identity operators we should tensor f with. We will thus allow ourselves to make this procedure implicit.

The idea will then be the following: for an operator f, its padded version f_{pad} will be defined as 'f tensored with the identity operators required to make its action meaningful, in the context of the expression at hand'. For instance, taking f to act on $\mathcal{H}_A \otimes \mathcal{H}_B$, and g to act on $\mathcal{H}_B \otimes \mathcal{H}_C$, $g_{\text{pad}} \circ f_{\text{pad}}$ will be taken to mean $(I_A \otimes g) \circ (f \otimes I_C)$, an operator acting on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$. For another example, taking h acting on $\mathcal{H}_C \otimes \mathcal{H}_D$, the equation $g_{\text{pad}} \circ f_{\text{pad}} = h_{\text{pad}}$ will be taken to mean $(I_A \otimes g \otimes I_D) \circ (f \otimes I_C \otimes I_D) = I_A \otimes I_B \otimes I_C \otimes h$. This notation will extend to supermaps as well: for instance, if $\mathcal{S}$ is a supermap of type $(\mathcal{H}_A^{\text{in}} \rightarrow \mathcal{H}_A^{\text{out}}) \rightarrow (\mathcal{H}_P \rightarrow \mathcal{H}_F)$, we will define its action on a map $f : \mathcal{H}_A^{\text{in}} \otimes \mathcal{H}_B^{\text{in}} \rightarrow \mathcal{H}_A^{\text{out}} \otimes \mathcal{H}_B^{\text{out}}$ as $\mathcal{S}_{\text{pad}}[f]$, which should be understood as $(\mathcal{S} \otimes \mathcal{I})[f]$, where $\mathcal{I}$ is the identity supermap on $\mathcal{L}(\mathcal{H}_B^{\text{in}} \rightarrow \mathcal{H}_B^{\text{out}})$.

Another related technique we will use in order to avoid clutter is to disregard the ordering of factors. Indeed, factors in a given tensor product are usually regarded as being labelled by ordered lists, rather than by sets, of indices. For instance, $\mathcal{H}_A \otimes \mathcal{H}_B$ and $\mathcal{H}_B \otimes \mathcal{H}_A$ are usually regarded as different (albeit isomorphic) spaces. Accordingly, suppose we take a map h over $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ which decomposes as a tensor product of a map f on $\mathcal{H}_A \otimes \mathcal{H}_C$ and a map g on $\mathcal{H}_B$. This fact, in the usual picture, could not be expressed as $h = f \otimes g$, as the RHS there acts on $\mathcal{H}_A \otimes \mathcal{H}_C \otimes \mathcal{H}_B$. Rather, one should write $h = (I \otimes \text{swap}_{C,B}) \circ (f \otimes g) \circ (I \otimes \text{swap}_{B,C})$. Another feature of the standard view is that it is not possible to write $\bigotimes_{X \in \{A,B\}} \mathcal{H}_X$, as this expression would leave the order of the factors ambiguous.

For the expressions we will consider, keeping with this use would force us to 1) explicitly introduce arbitrary orderings of all the sets of indices we use to label factors in tensor products, and 2) overload our expressions with swaps, in order to always place next to each other the spaces on which a given map acts. This would

once again create a lot of clutter with little relevance. We will therefore abstain ourselves from that constraint, and take the view that tensor products are labelled with sets, rather than ordered lists, of indices. This will allow us to write $h = f \otimes g$ in the case described above, or to write Hilbert spaces of the form $\otimes_{X \in \{A,B\}} \mathcal{H}_X$. The expressions we will write in this way could always be recast in the standard view, using arbitrary orderings of the sets at hand and large amounts of swaps.

One might wonder whether either padding or disregarding the ordering of factors might lead to ambiguities. In fact, such ambiguities only arise if some Hilbert spaces in a tensor product are labelled with the same index, for instance if one is dealing with a Hilbert space like $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A$. This is why we will carefully avoid such situations, by only ever tensoring different – although possibly isomorphic – Hilbert spaces. For instance, if we need a tensor product of $\mathcal{H}_A$ with itself, we will write it as $\mathcal{H}_A \otimes \mathcal{H}_{A'}$, with $\mathcal{H}_A \cong \mathcal{H}_{A'}$.

Note that the same techniques and notations will be used for relations.

C.2.2 Technical definitions on supermaps

Definition C.2.1 (Superrelation). *A superrelation of type $\bigtimes_N (K_N \to L_N) \to (P \to F)$, where P, F, the K_N's and the L_N's are all sets, is a relation $\mathcal{S}^{\textbf{Rel}} : \textbf{Rel}(\bigtimes_N K_N, \bigtimes_{N'} L_{N'}) \to \textbf{Rel}(P, F)$. With a slight abuse of notation, we denote $\mathcal{S}^{\textbf{Rel}}[(\lambda_N)_N] := \mathcal{S}^{\textbf{Rel}}[\bigotimes_N \lambda_N]$.*

Definition C.2.2 (Supermap). *A supermap of type $\bigtimes_N (\mathcal{H}_N^{\text{in}} \to \mathcal{H}_N^{\text{out}}) \to (\mathcal{H}_P \to \mathcal{H}_F)$, where $\mathcal{H}_P$, $\mathcal{H}_F$, the $\mathcal{H}_N^{\text{in}}$'s and the $\mathcal{H}_N^{\text{out}}$'s are all finite-dimensional Hilbert spaces, is a linear map $\mathcal{S} : \mathcal{L}(\bigotimes_N \mathcal{H}_N^{\text{in}}, \bigotimes_{N'} \mathcal{H}_{N'}^{\text{out}}) \to \mathcal{L}(\mathcal{H}_P, \mathcal{H}_F)$. With a slight abuse of notation, we denote $\mathcal{S}[(f_N)_N] := \mathcal{S}[\bigotimes_N f_N]$.*

Definition C.2.3 (Superunitary). *A superunitary of type $\bigtimes_N (\mathcal{H}_N^{\text{in}} \to \mathcal{H}_N^{\text{out}}) \to (\mathcal{H}_P \to \mathcal{H}_F)$ is a supermap of the same type such that, for any choice of ancillary input and output spaces $\mathcal{H}_N^{\text{in,anc}}$ and $\mathcal{H}_N^{\text{out,anc}}$ at every N, and any choice of unitary maps $U_N : \mathcal{H}_N^{\text{in}} \otimes \mathcal{H}_N^{\text{in,anc}} \to \mathcal{H}_N^{\text{out}} \otimes \mathcal{H}_N^{\text{out,anc}}$ at every N, one has:*

$$\mathcal{S}_{\text{pad}}[(U_N)_N] \text{ is a unitary from } \mathcal{H}_P \otimes \left(\bigotimes_N \mathcal{H}_N^{\text{in,anc}} \right) \text{ to } \mathcal{H}_F \otimes \left(\bigotimes_N \mathcal{H}_N^{\text{out,anc}} \right) . \quad \text{(C.12)}$$

Definition C.2.4 (Routed Supermap). *A routed supermap of type $\bigtimes_N (\mathcal{H}_N^{\text{in}} \overset{\lambda_N}{\to} \mathcal{H}_N^{\text{out}}) \to (\mathcal{H}_P \overset{\mu}{\to} \mathcal{H}_F)$, where the $\mathcal{H}_N^{\text{in}}$'s and the $\mathcal{H}_N^{\text{out}}$'s are sectorised finite-dimensional Hilbert spaces and the λ_N's are relations $\text{Ind}_N^{\text{in}} \to \text{Ind}_N^{\text{out}}$, is a supermap: i) which is restricted to only act on the maps of $\mathcal{L}(\bigotimes_N \mathcal{H}_N^{\text{in}}, \bigotimes_{N'} \mathcal{H}_{N'}^{\text{out}})$ that follow the route $\bigtimes_N \lambda_N$; and ii) whose output always follows the route μ.*

We say it is superunitary if it satisfies (C.12) when acting on routed unitaries $U_N : \mathcal{H}_N^{\text{in}} \otimes \mathcal{H}_N^{\text{in,anc}} \overset{\lambda_N}{\to} \mathcal{H}_N^{\text{out}} \otimes \mathcal{H}_N^{\text{out,anc}}$ that follow the routes.

C.2.3 Technical presentation of the framework

Definition C.2.5 (Indexed graph). *An* indexed graph Γ *consists of*

- *a finite set of nodes (or vertices)* Nodes_Γ;

- *a finite set of arrows (or edges)* $\mathrm{Arr}_\Gamma = \mathrm{Arr}_\Gamma^{\mathrm{in}} \sqcup \mathrm{Arr}_\Gamma^{\mathrm{int}} \sqcup \mathrm{Arr}_\Gamma^{\mathrm{out}}$;

- *functions* $\mathrm{head} : \mathrm{Arr}_\Gamma^{\mathrm{in}} \sqcup \mathrm{Arr}_\Gamma^{\mathrm{int}} \to \mathrm{Nodes}_\Gamma$ *and* $\mathrm{tail} : \mathrm{Arr}_\Gamma^{\mathrm{int}} \sqcup \mathrm{Arr}_\Gamma^{\mathrm{out}} \to \mathrm{Nodes}_\Gamma$;

- *for each arrow* $A \in \mathrm{Arr}_\Gamma$, *a finite set of indices* Ind_A, *satisfying:* $A \notin \mathrm{Arr}_\Gamma^{\mathrm{int}} \implies \mathrm{Ind}_A$ *is trivial (i.e. is a singleton);*

- *a function* $\mathrm{dim} : \bigsqcup_{A \in \mathrm{Arr}_\Gamma} \mathrm{Ind}_A \to \mathbb{N}^*$.

We further define $\mathrm{Ind}_\Gamma^{\mathrm{in}} := \bigtimes_{A \in \mathrm{Arr}_\Gamma^{\mathrm{in}}} \mathrm{Ind}_A$, $\mathrm{Ind}_\Gamma^{\mathrm{out}} := \bigtimes_{A \in \mathrm{Arr}_\Gamma^{\mathrm{out}}} \mathrm{Ind}_A$, and for any $N \in \mathrm{Nodes}_\Gamma$: $\mathrm{in}(N) := \mathrm{head}^{-1}(N)$, $\mathrm{out}(N) := \mathrm{tail}^{-1}(N)$, $\mathrm{Ind}_N^{\mathrm{in}} := \bigtimes_{A \in \mathrm{in}(N)} \mathrm{Ind}_A$ and $\mathrm{Ind}_N^{\mathrm{out}} := \bigtimes_{A \in \mathrm{out}(N)} \mathrm{Ind}_A$.

To prepare for the interpretation of this graph in terms of complex linear maps, we also define the following sectorised Hilbert spaces: for all $A \in \mathrm{Arr}_\Gamma$, $\mathcal{H}_A := \bigoplus_{k \in \mathrm{Ind}_A} \mathcal{H}_A^k$, where $\mathcal{H}_A^k \cong \mathbb{C}^{\mathrm{dim}(k)}$; $\mathcal{H}_P := \bigotimes_{A \in \mathrm{Arr}_\Gamma^{\mathrm{in}}} \mathcal{H}_A = \bigoplus_{\vec{k} \in \mathrm{Ind}_\Gamma^{\mathrm{in}}} \bigotimes \mathcal{H}_A^{k_A}$ and $\mathcal{H}_F := \bigotimes_{A \in \mathrm{Arr}_\Gamma^{\mathrm{out}}} \mathcal{H}_A = \bigoplus_{\vec{k} \in \mathrm{Ind}_\Gamma^{\mathrm{out}}} \bigotimes \mathcal{H}_A^{k_A}$; and for all $N \in \mathrm{Nodes}_\Gamma$, $\mathcal{H}_N^{\mathrm{in}} := \bigotimes_{A \in \mathrm{in}(N)} \mathcal{H}_A = \bigoplus_{\vec{k} \in \mathrm{Ind}_N^{\mathrm{in}}} \bigotimes \mathcal{H}_A^{k_A}$ and $\mathcal{H}_N^{\mathrm{out}} := \bigotimes_{A \in \mathrm{out}(N)} \mathcal{H}_A = \bigoplus_{\vec{k} \in \mathrm{Ind}_N^{\mathrm{out}}} \bigotimes \mathcal{H}_A^{k_A}$.

Definition C.2.6 (Branched relation). *A relation $\lambda : K \to L$ is said to be* branched *if, when seen as a function $K \to \mathcal{P}(L)$, it satisfies*

$$\forall k, k' \in K, \lambda(k) \cap \lambda(k') = \lambda(k) \text{ or } \emptyset, \tag{C.13}$$

i.e. $\lambda(k)$ and $\lambda(k')$ are disjoint or the same.

Note that λ is branched if and only if $\lambda^\top$ is branched. Branched relations define compatible, non-complete partitions of their domain and codomain, corresponding to *branches*. Formally, a branch α of the branched relation $\lambda : K \to L$ is a pair of non-empty sets $K^\alpha \subseteq K$ and $L^\alpha \subseteq L$ such that $\lambda(K^\alpha) = L^\alpha$ and $\lambda^\top(L^\alpha) = K^\alpha$. We denote the set of branches of λ as $\mathrm{Bran}(\lambda)$. Note that the partitions are not complete, i.e. $\bigsqcup_{\alpha \in \mathrm{Bran}(\lambda)} K^\alpha$ might not be equal to K (and the same goes for the outputs); the discrepancy corresponds to the indices that are sent by λ to the empty set, as we consider these indices to be part of no branch at all.

Definition C.2.7 (Routed graph). *A* routed graph $(\Gamma, (\lambda_N)_{N \in \mathrm{Nodes}_\Gamma})$ *consists of an indexed graph Γ and, for every node N, of a branched relation $\lambda : \mathrm{Ind}_N^{\mathrm{in}} \to \mathrm{Ind}_N^{\mathrm{out}}$, called the* route for node N.

We will write routed graphs as $(\Gamma, (\lambda_N)_N)$ for brevity. We denote elements of $\mathrm{Bran}(\lambda_N)$ as N^α, and denote the set of input (resp. output) indices of N^α as $\mathrm{Ind}_{N^\alpha}^{\mathrm{in}} \subseteq \mathrm{Ind}_N^{\mathrm{in}}$ (resp. $\mathrm{Ind}_{N^\alpha}^{\mathrm{out}} \subseteq \mathrm{Ind}_N^{\mathrm{out}}$). We also define $\mathrm{Bran}_{(\Gamma, (\lambda_N)_N)} := \bigsqcup_{N \in \mathrm{Nodes}_\Gamma} \mathrm{Bran}(\lambda_N)$, the set of all branches in the whole routed graph.

We will now define the notion of a branch being a *strong parent* of another: this will correspond to solid arrows in the branch graph. First, we introduce the set of possible tuple of values of indices, in order to exclude inconsistent assignments of values.

Definition C.2.8. *We define* $\mathtt{PossVal}_\Gamma$ *as the subset of* $\bigtimes_{A \in \mathtt{Arr}_\Gamma} \mathtt{Ind}_A$ *defined by*

$$\forall (k_A)_{A \in \mathtt{Arr}_\Gamma} \in \mathtt{PossVal}_\Gamma, \forall N \in \mathtt{Nodes}_\Gamma, \ (k_A)_{A \in \mathrm{in}(N)} \overset{\lambda_N}{\sim} (k_A)_{A \in \mathrm{out}(N)}. \tag{C.14}$$

A tuple of values is possible if and only if for every node, it yields a input and an output values that are in the same branch.

Lemma C.2.1. *Let* $\vec{k} = (k_A)_{A \in \mathtt{Arr}_\Gamma} \in \bigtimes_{A \in \mathtt{Arr}_\Gamma} \mathtt{Ind}_A$. $\vec{k} \in \mathtt{PossVal}_\Gamma$ *if and only if it meets the following two conditions:*

- $\forall N \in \mathtt{Nodes}_\Gamma$, $(k_A)_{A \in \mathrm{in}(N)}$ *is in* λ_N*'s practical inputs and* $(k_A)_{A \in \mathrm{out}(N)}$ *is in* λ_N*'s practical outputs;*

- *denoting, for every* N, $\mu_N^{\mathrm{in}}(\vec{k})$ *as the element of* $\mathtt{Bran}_N$ *such that* $(k_A)_{A \in \mathrm{in}(N)} \in \mathtt{Ind}^{\mathrm{in}}_{N^{\mu_N^{\mathrm{in}}(\vec{k})}}$, *and* $\mu_N^{\mathrm{out}}(\vec{k})$ *similarly, we have:* $\forall N, \mu_N^{\mathrm{in}}(\vec{k}) = \mu_N^{\mathrm{out}}(\vec{k})$.

Proof. This derives directly from the structure of the routes: a branched route relates an input value to an output value if and only if they are both in the same branch (and in particular, are not outside of its practical in/outputs). ☐

For $\vec{k} \in \mathtt{PossVal}_\Gamma$, we can therefore denote for every N the branch $\mu_N\left(\vec{k}\right)$ equal to both $\mu_N^{\mathrm{in}}(\vec{k})$ and $\mu_N^{\mathrm{out}}(\vec{k})$.

Definition C.2.9 (Strong parents). *Let* $(\Gamma, (\lambda_N)_{N \in \mathtt{Nodes}_\Gamma})$ *be a routed graph, and* N^α *and* M^β *two branches in it. We define the set of arrows from* N *to* M *as* $\mathtt{Link}(N, M) := \mathrm{out}(N) \cap \mathrm{in}(M)$. *We define* $\mathtt{LinkVal}(N^\alpha, M^\beta)$, *the set of values linking* N^α *to* M^β, *as*

$$\mathtt{LinkVal}(N^\alpha, M^\beta) := \left\{ (k_A)_{A \in \mathtt{Link}(N,M)} \middle| \exists (k_A)_{A \in \mathtt{Arr}_\Gamma \setminus \mathtt{Link}(N,M)} \text{ such that } \begin{cases} \mu_N\left((k_A)_{A \in \mathtt{Arr}_\Gamma}\right) = \alpha \\ \mu_M\left((k_A)_{A \in \mathtt{Arr}_\Gamma}\right) = \beta \end{cases} \right\} \tag{C.15}$$

We say that the branch N^α *is* not *a strong parent of the branch* M^β *if at least one of the following holds:*

- $\mathtt{Link}(N, M) = \varnothing$;

- $\mathtt{LinkVal}(N^\alpha, M^\beta) = \varnothing$;

- $\mathtt{LinkVal}(N^\alpha, M^\beta)$ *is a singleton and its unique element* $(k_A)_{A \in \mathtt{Link}(N,M)}$ *satisfies* $\forall A \in \mathtt{Link}(N, M), \dim(k_A) = 1$.

Definition C.2.10 (Adjoint of a graph). *If Γ is an indexed graph, its* adjoint $\Gamma^\top$ *is the indexed graph given by swapping the roles of* $\mathtt{Arr}_\Gamma^{\mathrm{in}}$ *and* $\mathtt{Arr}_\Gamma^{\mathrm{out}}$ *and those of* head *and* tail, *and leaving the rest invariant.*

If $(\Gamma, (\lambda_N)_N)$ is a routed graph, its adjoint is the routed graph $(\Gamma^\top, (\lambda_N{}^\top)_N)$.

Definition C.2.11 (Skeletal superrelation of an indexed graph). *Given an indexed graph Γ, its associated* skeletal superrelation *is the superrelation* $\mathcal{S}_\Gamma^{\mathbf{Rel}} : \bigtimes_N(\mathtt{Ind}_N^{\mathrm{in}} \to \mathtt{Ind}_N^{\mathrm{out}}) \to (\mathtt{Ind}_\Gamma^{\mathrm{in}} \to \mathtt{Ind}_\Gamma^{\mathrm{out}})$ *defined by*

$$\mathcal{S}_\Gamma^{\mathbf{Rel}}[(\lambda_N)_N] := \mathrm{Tr}_{\mathtt{Ind}_A, A \in \mathtt{Arr}_\Gamma^{\mathrm{int}}} \left[\bigotimes_N \lambda_N \right]. \tag{C.16}$$

Note that this is well-typed because $\bigtimes_N \mathtt{Ind}_N^{\mathrm{in}} = \bigtimes_{A \in \mathtt{Arr}_\Gamma^{\mathrm{in}} \sqcup \mathtt{Arr}_\Gamma^{\mathrm{int}}} \mathtt{Ind}_A$ *and* $\bigtimes_N \mathtt{Ind}_N^{\mathrm{out}} = \bigtimes_{A \in \mathtt{Arr}_\Gamma^{\mathrm{out}} \sqcup \mathtt{Arr}_\Gamma^{\mathrm{int}}} \mathtt{Ind}_A$.

Definition C.2.12 (Skeletal supermap of a routed graph). *Given a routed graph $(\Gamma, (\lambda_N)_N)$, its associated (routed)* skeletal supermap *is the supermap* $\mathcal{S}_{(\Gamma, (\lambda_N)_N)}$ *of type* $\bigtimes_N(\mathcal{H}_N^{\mathrm{in}} \xoverset{\lambda_N}{\to} \mathcal{H}_N^{\mathrm{out}}) \to (\mathcal{H}_P \xoverset{\mathcal{S}_\Gamma^{\mathbf{Rel}}[(\lambda_N)_N]}{\to} \mathcal{H}_F)$ *defined by*

$$\mathcal{S}_{(\Gamma, (\lambda_N)_N)}[(f_N)_N] := \mathrm{Tr}_{\mathcal{H}_A, A \in \mathtt{Arr}_\Gamma^{\mathrm{int}}} \left[\bigotimes_N f_N \right]. \tag{C.17}$$

Note that the fact that $\mathcal{S}_{(\Gamma, (\lambda_N)_N)}[(f_N)_N]$ follows the route $\mathcal{S}_\Gamma^{\mathbf{Rel}}[(\lambda_N)_N]$ when the f_N's follow the λ_N's is ensured by the fact that routed maps form a compact closed category [1, 4].

Definition C.2.13 (Augmented relation). *Given a relation $\lambda_N : \mathtt{Ind}_N^{\mathrm{in}} \to \mathtt{Ind}_N^{\mathrm{out}}$ serving as a route for node N, its* augmented *version is the partial function (encoded as a relation) $\lambda_N^{\mathrm{aug}} : \mathtt{Ind}_N^{\mathrm{in}} \times \left(\bigtimes_{\alpha \in \mathtt{Bran}(\lambda_N)} \mathtt{Ind}_{N^\alpha}^{\mathrm{out}} \right) \to \mathtt{Ind}_N^{\mathrm{out}} \times \left(\bigtimes_{\alpha \in \mathtt{Bran}(\lambda_N)} \mathtt{Happens}_{N^\alpha} \right)$ – where $\forall \alpha, \mathtt{Happens}_{N^\alpha} \cong \{0, 1\}$ – given by*

$$\lambda_N^{\mathrm{aug}}(k, (l^\alpha)_{\alpha \in \mathtt{Bran}(\lambda_N)}) = \begin{cases} \{(l^\alpha, (\delta_{\alpha'}^\alpha)_{\alpha \in \mathtt{Bran}(\lambda_N)})\} & \text{if } k \in \mathtt{Ind}_{N^\alpha}^{\mathrm{in}} \\ \varnothing & \text{if } \forall \alpha, k \notin \mathtt{Ind}_{N^\alpha}^{\mathrm{in}}. \end{cases} \tag{C.18}$$

Definition C.2.14 (Univocality). *A routed graph $(\Gamma, (\lambda_N)_N)$ is* univocal *if*

$$\mathcal{S}_{\Gamma, \mathrm{pad}}^{\mathbf{Rel}} \left[(\lambda_N^{\mathrm{aug}})_N \right] \text{ is a function.} \tag{C.19}$$

We then note this function as $\Lambda_{(\Gamma, (\lambda_N)_N)}$.

$(\Gamma, (\lambda_N)_N)$ is bi-univocal *if both it and its adjoint $\left(\Gamma^\top, (\lambda_N{}^\top)_N \right)$ are univocal.*

Definition C.2.15 (Branch graph). *If $(\Gamma, (\lambda_N)_N)$ is a bi-univocal routed graph, its* branch graph $\Gamma^{\mathtt{Bran}}$ *is the graph in which*

- *the nodes are the branches of $(\Gamma, (\lambda_N)_N)$, i.e. the elements of $\mathtt{Bran}_{(\Gamma, (\lambda_N)_N)}$;*

- *there is a green dashed arrow from N^α to M^β if $\Lambda_{(\Gamma, (\lambda_N)_N)}$ features influence from $\mathtt{Ind}_{N^\alpha}^{\mathrm{out}}$ to $\mathtt{Happens}_{M^\beta}$;*

- *there is a red dashed arrow from N^α to M^β if $\Lambda_{\left(\Gamma^\top, (\lambda_N{}^\top)_N\right)}$ features influence from $\text{Ind}^{\text{in}}_{M^\beta}$ to $\text{Happens}_{N^\alpha}$;*

- *there is a solid arrow from N^α to M^β if N^α is a strong parent of M^β.*

Definition C.2.16 (Weak loops). *Let $(\Gamma, (\lambda_N)_N)$ be a bi-univocal routed graph. We say that a loop in Γ^{Bran} is* weak *if it only contains green dashed arrows, or if it only contains red dashed arrows.*

Theorem C.2.1 (Main theorem). *Let $(\Gamma, (\lambda_N)_N)$ be a routed graph which is bi-univocal, and whose branch graph Γ^{Bran} only features weak loops. Then its associated skeletal supermap $\mathcal{S}_{(\Gamma, (\lambda_N)_N)}$ is a superunitary.*

The rest of this Appendix is dedicated to the proof of this theorem.

C.2.4 Proof

Preliminary lemmas and definitions

Lemma C.2.2. *To prove Theorem C.2.1, it is sufficient to prove that, for any valid routed graph $(\Gamma, (\lambda_N)_N)$, $\mathcal{S}_{(\Gamma, (\lambda_N)_N)}$ preserves unitarity when acting on input operations without ancillas.*

Proof. Suppose it was proven that for any valid $(\Gamma, (\lambda_N)_N)$, and for any set of routed unitaries $U_N : \mathcal{H}^{\text{in}}_N \overset{\lambda_N}{\to} \mathcal{H}^{\text{out}}_N$, $\mathcal{S}_{(\Gamma, (\lambda_N)_N)}[(U_N)_N]$ is a unitary.

Taking now a valid $(\Gamma, (\lambda_N)_N)$ and, for every N, a choice of ancillary input and output spaces $\mathcal{H}^{\text{in,anc}}_N$ and $\mathcal{H}^{\text{out,anc}}_N$, and a routed unitary $U_N : \mathcal{H}^{\text{in}}_N \otimes \mathcal{H}^{\text{in,anc}}_N \overset{\lambda_N}{\to} \mathcal{H}^{\text{out}}_N \otimes \mathcal{H}^{\text{out,anc}}_N$. One can then define a new indexed graph $\tilde{\Gamma}$ by adding, for each N, a new arrow in $\text{Arr}^{\text{in}}_\Gamma$, with Hilbert space $\mathcal{H}^{\text{in,anc}}_N$, and a new arrow in $\text{Arr}^{\text{out}}_\Gamma$, with Hilbert space $\mathcal{H}^{\text{out,anc}}_N$. The routed graph $(\tilde{\Gamma}, (\lambda_N)_N)$ then has the same choice relation and the same branch graph as $(\Gamma, (\lambda_N)_N)$; it is therefore valid as well. We can thus apply our assumption to it, which entails that $\mathcal{S}_{(\tilde{\Gamma}, (\lambda_N)_N)}[(U_N)_N] = \mathcal{S}^{\text{pad}}_{(\Gamma, (\lambda_N)_N)}[(U_N)_N]$ is unitary. This thus proves the theorem in the general case. □

From now on, we will therefore work with a fixed routed graph $(\Gamma, (\lambda_N)_N)$ (which we will often denote as Γ for simplicity) satisfying bi-univocality and weak loops, and a fixed collection of routed unitary maps $U_N : \mathcal{H}^{\text{in}}_N \overset{\lambda_N}{\to} \mathcal{H}^{\text{out}}_N$ following the λ_N's. Writing $\mathcal{S} := \mathcal{S}_{(\Gamma, (\lambda_N)_N)}$ for simplicity, our goal is to prove that $\mathcal{S}[(U_N)_N] : \mathcal{H}_P \to \mathcal{H}_F$ is a unitary.

For each branch N^α, we define $\mathcal{H}^{\text{in}}_{N^\alpha} := \bigoplus_{(k_A)_{A \in \text{in}(N)} \in \text{Ind}^{\text{in}}_{N^\alpha}} \bigotimes_{A \in \text{in}(N)} \mathcal{H}^{k_A}_A \subseteq \mathcal{H}^{\text{in}}_N$, $\mathcal{H}^{\text{out}}_{N^\alpha} := \bigoplus_{(k_A)_{A \in \text{out}(N)} \in \text{Ind}^{\text{out}}_{N^\alpha}} \bigotimes_{A \in \text{out}(N)} \mathcal{H}^{k_A}_A \subseteq \mathcal{H}^{\text{out}}_N$. We also define the projection $p^\alpha_N : \mathcal{H}^{\text{in}}_N \to \mathcal{H}^{\text{in}}_{N^\alpha}$ and the injection $i^\alpha_N : \mathcal{H}^{\text{out}}_{N^\alpha} \to \mathcal{H}^{\text{out}}_N$.

We define the *exchange* gate for N, $\text{EXCH}_N : \mathcal{H}^{\text{in}}_N \otimes \left(\bigotimes_{\alpha \in \text{Bran}(\lambda_N)} \mathcal{H}^{\text{out}}_{N^\alpha} \right) \to \mathcal{H}^{\text{out}} \otimes \left(\bigotimes_{\alpha \in \text{Bran}(\lambda_N)} \mathcal{H}^{\text{in}}_{N^\alpha} \right)$, by

$$\text{EXCH}_N := \sum_{\alpha \in \text{Bran}(\lambda_N)} i^\alpha_{N,\text{pad}} \circ \left(\text{SWAP}_{N^\alpha_{\text{in}}, N^\alpha_{\text{out}}} \otimes \left(\bigotimes_{\beta \neq \alpha} \Theta_{N^\beta} \right) \right) \circ p^\alpha_{N,\text{pad}}, \tag{C.20}$$

where $\forall N^\beta, \Theta_{N^\beta}$ is an arbitrarily chosen unitary from $\mathcal{H}^{\text{out}}_{N^\beta}$ to $\mathcal{H}^{\text{in}}_{N^\beta}$. Note that EXCH_N follows λ_N by construction.

We note that the fact that the U_N's follow the λ_N's entails that one can find a block decomposition for them, i.e., one can define unitaries $U^\alpha_N : \mathcal{H}^{\text{in}}_{N^\alpha} \to \mathcal{H}^{\text{out}}_{N^\alpha}$ such that

$$\forall N, U_N = \sum_{\alpha \in \text{Bran}(\lambda_N)} i^\alpha_{N,\text{pad}} \circ U^\alpha_N \circ p^\alpha_{N,\text{pad}}. \tag{C.21}$$

As a first preliminary to the proof, we will study in detail how bifurcation choices are in correspondence with assignments of values to the arrow's indices.

The following definition and lemma prove two things. First, univocality implies that any tuple of bifurcation choices fixes not only the branch at every node, but also the specific index values picked in that branch. Second, for a fixed tuple of bifurcation choices, the bifurcation choices at the branches not happening have no effect – i.e. modifying them to any other value wouldn't affect the any of the index values in the graph; while, on the contrary, modifying the bifurcation choice at any of the branches happening always changes at least one of the index values in the graph. In that sense, any tuple of values of the graph's indices corresponds either to no tuple of bifurcation choices at all, or to exactly one bifurcation choice at the branches that happen for this tuple of values, with no dependence on the bifurcation choices at branches that don't happen.

Definition C.2.17. *For every N in* Nodes_Γ*, we take* $\text{Ind}^{\text{out}\prime}_N \cong \text{Ind}^{\text{out}}_N$ *and define the partial function (encoded as a relation)* $\lambda^{\text{sec}}_N : \text{Ind}^{\text{in}}_N \times \left(\times_{\alpha \in \text{Bran}_N} \text{Ind}^{\text{out}}_{N^\alpha} \right) \to \text{Ind}^{\text{out}}_N \times \text{Ind}^{\text{out}\prime}_N$ *given by*

$$\lambda^{\text{sec}}_N(k, (l^\alpha)_{\alpha \in \text{Bran}_N}) = \begin{cases} \{(l^\alpha, l^\alpha)\} & \text{if } k \in \text{Ind}^{\text{in}}_{N^\alpha} \\ \varnothing & \text{if } \forall \alpha, \, k \notin \text{Ind}^{\text{in}}_{N^\alpha}. \end{cases} \tag{C.22}$$

Lemma C.2.3. *If* $(\Gamma, (\lambda_N)_N)$ *is univocal, then* $\mathcal{S}^{\textbf{Rel}}\left[(\lambda^{\text{sec}}_N)_N\right]$ *is an injective function* $\times_{N^\alpha \in \text{Bran}_\Gamma} \text{Ind}^{\text{out}}_{N^\alpha} \to \times_N \text{Ind}^{\text{out}\prime}_N$*, which we denote* Λ^{sec}*. Furthermore, its preimage sets are given by*

$$\forall (k_N)_N, \, (\Lambda^{\text{sec}})^{-1}((k_N)_N) = \text{either } \varnothing \text{ or } \left(\times_N \{k_N\} \right) \times \left(\times_{N^\alpha | k_N \notin \text{Ind}^{\text{out}}_{N^\alpha}} \text{Ind}^{\text{out}}_{N^\alpha} \right). \tag{C.23}$$

Proof. We will use bra-ket notations for relational states and effects. For every branch N^α, we define $\text{COPY}_{N^\alpha_{\text{out}}} : \text{Ind}^{\text{out}}_{N^\alpha} \to \text{Ind}^{\text{out}}_{N^\alpha} \times \text{Ind}^{\text{out}\prime}_{N^\alpha}$, with $\text{Ind}^{\text{out}\prime}_{N^\alpha} \cong \text{Ind}^{\text{out}}_{N^\alpha}$, by

$\text{COPY}_{N_{\text{out}}^{\alpha}} |l\rangle = |l\rangle \otimes |l\rangle$. For every node N, we define the partial function (encoded as a relation) $\sigma^N : \bigtimes_{\alpha \in \text{Bran}(\lambda_N)} \text{Happens}_{N^{\alpha}} \to \text{Bran}_N$ by

$$\sigma^N((\varepsilon^{\alpha'})_{\alpha' \in \text{Bran}_N}) = \begin{cases} \{\alpha\} & \text{if } \forall \alpha', \varepsilon^{\alpha'} = \delta_\alpha^{\alpha'} \\ \varnothing & \text{otherwise.} \end{cases} \tag{C.24}$$

For every node N, we define the function $\nu^N : \text{Bran}_N \times \left(\bigtimes_{\alpha \in \text{Bran}_N} \text{Ind}_{N^{\alpha}}^{\text{out}\prime} \right) \to \text{Ind}_N^{\text{out}\prime}$, with $\text{Ind}_N^{\text{out}\prime} \cong \text{Ind}_N^{\text{out}}$, by

$$\nu^N(\vec{l}, \alpha) = l^{\alpha}. \tag{C.25}$$

One can then compute that $\lambda_N^{\text{sec}} = \nu_{\text{pad}}^N \circ \sigma_{\text{pad}}^N \circ \lambda_{N,\text{pad}}^{\text{aug}} \circ \text{COPY}_{N_{\text{out}}^{\alpha},\text{pad}}$; we can thus re-express Λ^{sec} in terms of the choice function Λ,

$$\Lambda^{\text{sec}} = \mathcal{S}^{\mathbf{Rel}}[(\lambda_N^{\text{sec}})_N] = \left(\prod_N \nu_{\text{pad}}^N \right) \circ \left(\prod_N \sigma_{\text{pad}}^N \right) \circ \Lambda \circ \left(\prod_{N^{\alpha}} \text{COPY}_{N_{\text{out}}^{\alpha},\text{pad}} \right). \tag{C.26}$$

Given that the outputs of a λ_N^{aug} are within the domain of definition of the corresponding σ^N, the fact that Λ is a function thus implies that $\left(\prod_N \sigma_{\text{pad}}^N \right) \circ \Lambda$ is a function as well. Given that the $\text{COPY}_{N_{\text{out}}^{\alpha}}$'s and ν^N's are functions, Λ^{sec} is a function as well.

Furthermore, let us fix an N and $k_N \in \text{Ind}_N^{\text{out}}$. If k_N is outside of λ_N's practical outputs, it immediately has no preimage through ν^N. Taking the other case, we denote α as the branch of N such that $k_N \in \text{Ind}_{N^{\alpha}}^{\text{out}}$. Then,

$$\langle k_N |_{\text{Ind}_{N^{\alpha}}^{\text{out}\prime},\text{pad}} \circ \lambda_N^{\text{sec}}$$

$$= \langle k_N |_{\text{Ind}_{N^{\alpha}}^{\text{out}\prime},\text{pad}} \circ \nu_{\text{pad}}^N \circ \sigma_{\text{pad}}^N \circ \lambda_{N,\text{pad}}^{\text{aug}} \circ \left(\bigotimes_{\alpha' \in \text{Bran}_N} \text{COPY}_{N_{\text{out}}^{\alpha'}} \right)_{\text{pad}}$$

$$= \langle k_N |_{\text{Ind}_{N^{\alpha}}^{\text{out}\prime},\text{pad}} \circ \left(\bigotimes_{\alpha' \in \text{Bran}_N \setminus \{\alpha\}} \langle \text{Ind}_{N^{\alpha'}}^{\text{out}} | \right)_{\text{pad}} \circ \sigma_{\text{pad}}^N \circ \lambda_{N,\text{pad}}^{\text{aug}} \circ \left(\bigotimes_{\alpha' \in \text{Bran}_N} \text{COPY}_{N_{\text{out}}^{\alpha'}} \right)_{\text{pad}}$$

$$= \langle k_N |_{\text{Ind}_{N^{\alpha}}^{\text{out}\prime},\text{pad}} \circ \sigma_{\text{pad}}^N \circ \lambda_{N,\text{pad}}^{\text{aug}} \circ (\, |k_N\rangle \langle k_N| \,)_{\text{Ind}_{N^{\alpha}}^{\text{out}},\text{pad}}$$

$$= \left(\bigotimes_{\alpha' \in \text{Bran}_N} \langle \delta_\alpha^{\alpha'} |_{\text{Happens}_{N^{\alpha'}}} \right)_{\text{pad}} \circ \lambda_{N,\text{pad}}^{\text{aug}} \circ (\, |k_N\rangle \langle k_N| \,)_{\text{Ind}_{N^{\alpha}}^{\text{out}},\text{pad}}$$

$$= |k_N\rangle_{\text{Ind}_N^{\text{out}}} \left(\langle \text{Ind}_{N^{\alpha}}^{\text{in}} |_{\text{Ind}_N^{\text{in}}} \otimes \langle k_N |_{\text{Ind}_N^{\text{out}}} \otimes \left(\bigotimes_{\alpha' \in \text{Bran}_N \setminus \{\alpha\}} \langle \text{Ind}_{N^{\alpha'}}^{\text{out}} | \right) \right). \tag{C.27}$$

Therefore, we find that $(\Lambda^{\text{sec}})^{-1}((k_N)_N)$ is empty if at least one of the k_N's is outside of the practical outputs of the corresponding λ_N's, and that otherwise – denoting,

for every N, $\alpha(k_N)$ as the branch such that $k_N \in \mathrm{Ind}^{\mathrm{out}}_{N^{\alpha(k_N)}}-$,

$$
\left(\bigotimes_{N \in \mathrm{Nodes}_\Gamma} \langle k_N |_{\mathrm{Ind}^{\mathrm{out}\prime}_N} \right) \circ \Lambda^{\mathrm{sec}}
$$

$$
= \left(\bigotimes_{N \in \mathrm{Nodes}_\Gamma} \langle k_N |_{\mathrm{Ind}^{\mathrm{out}\prime}_N} \right) \circ \mathcal{S}^{\mathbf{Rel}} \left[(\lambda^{\mathrm{sec}}_N)_N \right]
$$

$$
= \mathcal{S}^{\mathbf{Rel}} \left[\left(| k_N \rangle_{\mathrm{Ind}^{\mathrm{out}}_N} \langle \mathrm{Ind}^{\mathrm{in}}_{N^{\alpha(k_N)}} |_{\mathrm{Ind}^{\mathrm{in}}_N} \right)_N \right] \otimes \left(\bigotimes_{N \in \mathrm{Nodes}_\Gamma} \langle k_N |_{\mathrm{Ind}^{\mathrm{out}}_{N^{\alpha(k_N)}}} \otimes \left(\bigotimes_{\alpha' \in \mathrm{Bran}_N \setminus \{\alpha(k_N)\}} \langle \mathrm{Ind}^{\mathrm{out}}_{N^{\alpha'}} | \right) \right) .
$$

$$\tag{C.28}$$

$\mathcal{S}^{\mathbf{Rel}} \left[\left(| k_N \rangle_{\mathrm{Ind}^{\mathrm{out}}_N} \langle \mathrm{Ind}^{\mathrm{in}}_{N^{\alpha(k_N)}} |_{\mathrm{Ind}^{\mathrm{in}}_N} \right)_N \right]$ is just a scalar in the theory of relations, i.e. 0 or 1; $(\Lambda^{\mathrm{sec}})^{-1} ((k_N)_N)$ is thus non-empty if and only if this scalar is equal to 1, and the rest of the expression yields (C.23). This also shows that $\Lambda^{\mathrm{sec}}_\Gamma$ is injective. $\qquad \square$

Note that we defined $\Lambda^{\mathrm{sec}}_\Gamma$ as having codomain $\times_{N \in \mathrm{Nodes}_\Gamma} \mathrm{Ind}^{\mathrm{out}}_N$; but, given that for each N we have $\mathrm{Ind}^{\mathrm{out}}_N = \times_{A \in \mathrm{out}(N)} \mathrm{Ind}_A$, we can also see it as a function to $\times_{A \in \mathrm{Arr}_\Gamma} \mathrm{Ind}_A$ (we neglect the discrepancy due to global input arrows of the graph, as their sets of index values are trivial). $\Lambda^{\mathrm{sec}}_\Gamma$ can thus be interpreted as telling us how bifurcation choices fix all indices in the graph. $\Lambda^{\mathrm{sec}}_{\Gamma^\top}$, obtained from considering the adjoint graph, tells us the same about reverse bifurcation choices.

From that perspective, in the above Lemma, the case of an empty set of preimages corresponds exactly to impossible assignments of values to the arrows, i.e. to ones that are outside of $\mathrm{PossVal}_\Gamma$.

Lemma C.2.4. *Given $\vec{k} = (k_A)_{A \in \mathrm{Arr}_\Gamma}$, $(\Lambda^{\mathrm{sec}})^{-1} (\vec{k})$ is empty if and only if $\vec{k} \notin \mathrm{PossVal}_\Gamma$.*

Proof. First, if there exists an N such that $k_N = (k_A)_{A \in \mathrm{out}(N)}$ is outside λ_N's practical outputs, then $(\Lambda^{\mathrm{sec}})^{-1} (\vec{k})$ is empty (as pointed out in the previous proof), and $\vec{k} \notin \mathrm{PossVal}_\Gamma$ (as pointed out in Lemma C.2.1).

Otherwise, we know from the previous proof that $(\Lambda^{\mathrm{sec}})^{-1} (\vec{k})$ is not empty if and only if $\mathcal{S}^{\mathbf{Rel}} \left[\left(| k_N \rangle_{\mathrm{Ind}^{\mathrm{out}}_N} \langle \mathrm{Ind}^{\mathrm{in}}_{N^{\alpha(k_N)}} |_{\mathrm{Ind}^{\mathrm{in}}_N} \right)_N \right] = 1$. But given how $\mathcal{S}^{\mathbf{Rel}}$ was defined in (C.16), and the form of the λ_N's, this is the case if and only if for all N, $(k_A)_{A \in \mathrm{in}(N)}$ is in the branch $\alpha(k_N)$. As the function α_N is precisely the function μ^{out}_N defined in Lemma C.2.1, we thus find the condition $\mu^{\mathrm{out}}_N(\vec{k}) = \mu^{\mathrm{in}}_N(\vec{k})$ showed in this Lemma to be necessary and sufficient for $\vec{k} \in \mathrm{PossVal}_\Gamma$. $\qquad \square$

Finally, we draw the consequences of the fact that branches satisfy the weak loops condition. Given a branch N^α, we define the following subsets of Bran_Γ. By a 'path' in $\Gamma^{\mathtt{Bran}}$, we mean any sequence of arrows, without a distinction between the solid, green dashed or red dashed types.

- $\mathcal{P}(N^\alpha) := \{O^\gamma \neq N^\alpha \mid \exists \text{ a path } O^\gamma \to N^\alpha \text{ in } \Gamma^{\texttt{Bran}}\}$, N^α's past;

- $\mathcal{F}(N^\alpha) := \{O^\gamma \neq N^\alpha \mid \exists \text{ a path } N^\alpha \to O^\gamma \text{ in } \Gamma^{\texttt{Bran}}\}$, N^α's future;

- $\mathcal{L}(N^\alpha) := \mathcal{P}(N^\alpha) \cap \mathcal{F}(N^\alpha)$, N^α's layer (i.e. the branches that form a loop with N^α);

- $\mathcal{P}^{\text{str}}(N^\alpha) := \mathcal{P}(N^\alpha) \setminus \mathcal{L}(N^\alpha)$, N^α's strict past;

- $\mathcal{F}^{\text{str}}(N^\alpha) := \mathcal{F}(N^\alpha) \setminus \mathcal{L}(N^\alpha)$, N^α's strict future;

It is clear that the relation $\sim$, defined by: $N^\alpha \sim O^\gamma$ if $N^\alpha = O^\gamma$ or $O^\gamma \in \mathcal{L}(N^\alpha)$, is an equivalence relation on $\texttt{Bran}_\Gamma$, partitioning it into a collection of layers. The fact that all loops in $\texttt{Bran}_\Gamma$ are weak then allows us to say that a given layer either only contains green dashed arrows between its elements (in which case we will call it a green layer), or only contains red dashed arrows (in which case we will call it a red layer).[2]

Furthermore, merging the nodes of each layer transforms $\Gamma^{\texttt{Bran}}$ into an acyclic graph. One can thus define a partial order between layers. Arbitrarily turning it into a total order, and picking arbitrary orderings within each layer, leads to a total ordering $<$ of $\texttt{Bran}_\Gamma$ in which branches of a same layer are all next to each other, and in which $N^\alpha < O^\gamma \implies N^\alpha \notin \mathcal{F}^{\text{str}}(O^\gamma)$. We can use this total ordering to label the branches with natural numbers, as $\texttt{Bran}_\Gamma = \{B(i) \mid 1 \leq i \leq n\}$. For a given i and a given branch $N^\alpha > B(i)$, we define $\mathcal{P}_i(N^\alpha) := \mathcal{P}(N^\alpha) \cap \{O^\gamma > B(i)\}$, $\mathcal{F}_i(N^\alpha) := \mathcal{F}(N^\alpha) \cap \{O^\gamma > B(i)\}$, etc.

The induction hypothesis

This ordering of Γ's branches will allows us to define an induction. The point is to start from $\mathcal{S}_{\text{pad}}[(\text{EXCH}_N)_N]$, and then to 'refill' the branches one by one, making sure that the unitary obtained at each step is sufficiently well-behaved to be able to move to the next step. To define it, we will first need to define these 'partially filled exchanges' that are being used at every step i in the induction, which we shall call $V_{N,i}$'s. We do so by defining how they act on each branch: i.e., $\forall i, \forall N^\alpha$, we define $V_{N,i}^\alpha : \mathcal{H}_N^{\text{in}} \otimes \left(\bigotimes_{\beta \mid N^\beta > B(i)} \mathcal{H}_{N^\beta}^{\text{out}} \right) \to \mathcal{H}_N^{\text{out}} \otimes \left(\bigotimes_{\beta \mid N^\beta > B(i)} \mathcal{H}_{N^\beta}^{\text{in}} \right)$ by

$$
V_{N,i}^\alpha =
\begin{cases}
i_{N,\text{pad}}^\alpha \circ \left(\text{SWAP}_{N_{\text{in}}^\alpha, N_{\text{out}}^\alpha} \otimes \left(\bigotimes_{\beta > B(i), \beta \neq \alpha} \Theta_{N^\beta} \right) \right) \circ p_{N,\text{pad}}^\alpha & \text{if } N^\alpha > B(i), \\
\left(i_N^\alpha \circ U_N^\alpha \circ p_N^\alpha \right) \otimes \left(\bigotimes_{\beta > B(i)} \Theta_{N^\beta} \right) & \text{if } N^\alpha \leq B(i),
\end{cases}
\tag{C.29}
$$

and we use them to define

$$
V_{N,i} := \sum_{\alpha \in \texttt{Bran}(\lambda_N)} V_{N,i}^\alpha . \tag{C.30}
$$

---

[2]Note that single-branch layers can be considered to be either green or red: the choice will not affect the proof.

We will write the input (resp. output) space of $\mathcal{S}_{\text{pad}}[(V_{N,i})_N]$ as $\mathcal{H}_i^{\text{out}} := \mathcal{H}_P \otimes \left(\otimes_{N^\beta > B(i)} \mathcal{H}_{N^\beta}^{\text{out}} \right)$ (resp. $\mathcal{H}_i^{\text{in}} := \mathcal{H}_F \otimes \left(\otimes_{N^\beta > B(i)} \mathcal{H}_{N^\beta}^{\text{in}} \right)$). We also write $\bar{V}_{N,i}^\alpha := V_{N,i} - V_{N,i}^\alpha$. Note that the $V_{N,i}$'s follow the λ_N's by construction, and that one has $V_{N,0} = \text{EXCH}_N$ and $V_{N,n} = U_N$.

The core of the induction will be the hypothesis that, at step i, $\mathcal{S}_{\text{pad}}[(V_{N,i})_N]$ is unitary. However, this will not be sufficient: we will also need other conditions ensuring that $\mathcal{S}_{\text{pad}}[(V_{N,i})_N]$ features structural properties which allow us to move to step $i+1$. More precisely, these conditions will encode the fact that at every step i, and for every branch N^α that hasn't been filled yet (i.e. such that $N^\alpha > B(i)$), one can find projectors on $\mathcal{S}_{\text{pad}}[(V_{N,i})_N]$'s inputs and outputs that control whether N^α happens or not, and that all these projectors will play well with one another.

One subtlety is that, if $B(i)$ is in a *red* layer and if there are still unfilled branches in that layer, then the projectors controlling the status of branches above that layer cannot be defined. This is ultimately not problematic, as one can wait for the whole layer to have been filled to redefine them; but this will force us to amend parts of the induction hypothesis when it is the case.

Finally, another part of the induction hypothesis will rely on the causal properties of $\mathcal{S}_{\text{pad}}[(V_{N,i})_N]$. We will describe these by using the behaviour of $\mathcal{S}_{\text{pad}}[(V_{N,i})_N]$ seen as an isomorphism of operator algebras, defining $\mathcal{V}_i : \text{Lin}\left[\mathcal{H}_P \otimes \left(\otimes_{O^\gamma > B(i)} \mathcal{H}_{O_{\text{out}}^\gamma} \right) \right] \rightarrow \text{Lin}\left[\mathcal{H}_F \otimes \left(\otimes_{O^\gamma > B(i)} \mathcal{H}_{O_{\text{in}}^\gamma} \right) \right]$ by

$$\forall f, \mathcal{V}_i[f] := \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \circ f \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N]^\dagger. \tag{C.31}$$

When $\mathcal{S}_{\text{pad}}[(V_{N,i})_N]$ is unitary, this defines an isomorphism of operator algebras, preserving sums, compositions, and the dagger. This implies that, more generally, $\mathcal{V}_i$ will preserve commutation relations, self-adjointness, idempotency, etc.

We now turn to our induction hypotheses at step i.

Induction Hypothesis 1 (H1). $\mathcal{S}_{\text{pad}}[(V_{N,i})_N]$ *is unitary.*

As we mentioned, H1 is the core of the induction, and will allow us to conclude in the end that $\mathcal{S}[(V_{N,n})_N] = \mathcal{S}[(U_N)_N]$ is indeed unitary.

Induction Hypothesis 2 (H2). *One has defined, for all $N^\alpha > B(i)$, orthogonal projectors:*

- $\zeta_i^{\text{out}}(N^\alpha)$, *acting on* $\begin{cases} \mathcal{H}_P \otimes \left(\otimes_{O^\gamma \in \mathcal{P}_i(N^\alpha)} \mathcal{H}_{O_{\text{out}}^\gamma} \right) & \text{if } N^\alpha \text{ is in a green layer;} \\ \mathcal{H}_P \otimes \left(\otimes_{O^\gamma \in \mathcal{P}_i^{\text{str}}(N^\alpha)} \mathcal{H}_{O_{\text{out}}^\gamma} \right) & \text{if } N^\alpha \text{ is in a red layer;} \end{cases}$

- $\zeta_i^{\text{in}}(N^\alpha)$, *acting on* $\begin{cases} \mathcal{H}_F \otimes \left(\otimes_{O^\gamma \in \mathcal{F}_i^{\text{str}}(N^\alpha)} \mathcal{H}_{O_{\text{in}}^\gamma} \right) & \text{if } N^\alpha \text{ is in a green layer;} \\ \mathcal{H}_F \otimes \left(\otimes_{O^\gamma \in \mathcal{F}_i(N^\alpha)} \mathcal{H}_{O_{\text{in}}^\gamma} \right) & \text{if } N^\alpha \text{ is in a red layer;} \end{cases}$

such that (once correctly padded) the $\zeta_{i,\text{pad}}^{\text{out}}(N^\alpha)$'s for different N^α's all commute pairwise, and the $\zeta_{i,\text{pad}}^{\text{in}}(N^\alpha)$'s commute as well, and such that

$$\forall N^\alpha, \ \zeta_{i,\text{pad}}^{\text{in}}(N^\alpha) = \mathcal{V}_i[\zeta_{i,\text{pad}}^{\text{out}}(N^\alpha)]. \tag{C.32}$$

If $B(i)$ and $B(i+1)$ are in the same red layer, then all of the former definitions have only been made for the N^α's in that same layer, i.e. in $\mathcal{L}_i(B(i))$. When this happens, we say that i is a special step.

H2 introduces the projectors that will be used to control the status of the still-unfilled branches. The fact that the ζ's commute pairwise ensures that these controls can always be meaningfully combined. Note that the out-projector for N^α only acts on N^α's past, while its in-projector only acts on N^α's future; and furthermore, that for N^α in a green layer its in-projector only acts on N^α's *strict* future, while for N^α in a red layer its out-projector only acts on its *strict* past. In particular, the $\zeta(N^\alpha)$'s never act on N^α itself: this ensures that at any step, a branch never holds some part of its own controls.

We will also write $\bar\zeta_i^{\text{in}}(N^\alpha) := \mathbb{1} - \zeta_i^{\text{in}}(N^\alpha)$ and $\bar\zeta_i^{\text{out}}(N^\alpha) := \mathbb{1} - \zeta_i^{\text{out}}(N^\alpha)$.

Induction Hypothesis 3 (H3)**.** *The ζ_i^{out}'s satisfy*

$$\forall N^\alpha, \forall O^\gamma, \zeta_{i,\text{pad}}^{\text{out}}(N^\alpha) \circ \bar\zeta_{i,\text{pad}}^{\text{out}}(O^\gamma) \text{ acts trivially on } \mathcal{H}_{O_{\text{out}}^\gamma}, \tag{C.33}$$

and the ζ_i^{in}'s satisfy

$$\forall N^\alpha, \forall O^\gamma, \zeta_{i,\text{pad}}^{\text{in}}(N^\alpha) \circ \bar\zeta_{i,\text{pad}}^{\text{in}}(O^\gamma) \text{ acts trivially on } \mathcal{H}_{O_{\text{in}}^\gamma}. \tag{C.34}$$

This hypothesis encodes the fact that, when a branch O^γ doesn't happen, it doesn't hold any control on other branches N^α. Note that the $\forall N^\alpha, O^\gamma$ only runs over the branches for which the ζ's have been defined in H2, i.e. it only runs over $\mathcal{L}_i(B(i))$ if i is a special step. The same will apply in the other hypotheses.

Induction Hypothesis 4 (H4)**.** *The ζ_i^{out}'s satisfy:*

$$\forall N^\alpha, N^\beta, \text{ branches of the same node, } \zeta_{i,\text{pad}}^{\text{out}}(N^\alpha) \circ \zeta_{i,\text{pad}}^{\text{out}}(N^\beta) = 0. \tag{C.35}$$

The meaning is that two branches of the same node are incompatible. Note that one can infer, using (C.32), that the ζ_i^{in}'s then satisfy the same property.

Induction Hypothesis 5 (H5)**.** *Let $Q \subseteq \{B(i') \mid i' \geq i\}$ a set of branches on different nodes; i.e., one can define $\tilde{Q} \subseteq \texttt{Nodes}_\Gamma$ and a function α such that $Q = \{N^{\alpha(N)} \mid N \in \tilde{Q}\}$. Then,*

$$\mathcal{S}_{\text{pad}}[(V_{N,i})_N] \circ \prod_{N \in \tilde{Q}} \zeta_{i,\text{pad}}^{\text{out}}\left(N^{\alpha(N)}\right) = \mathcal{S}_{\text{pad}}\left[(V_{N,i})_{N \in \texttt{Nodes}_\Gamma \setminus \tilde{Q}} \times \left(V_{N,i}^{\alpha(N)}\right)_{N \in \tilde{Q}}\right]. \tag{C.36}$$

H5 formalises the fact that the ζ_i^{out}'s control whether branches happen or not. Note that, using (C.32), one could have written the same equation using ζ_i^{in}'s.

Induction Hypothesis 6 (H6)**.** *For a branch N^α in a green layer, we have*

$$\forall f \in \text{Lin}[\mathcal{H}_{N^\alpha_{\text{in}}}], \exists f' \in \text{Lin}\left[\mathcal{H}_P \otimes \left(\bigotimes_{O^\gamma \in \mathcal{P}^{\text{str}}_i(N^\alpha)} \mathcal{H}_{O^\gamma_{\text{out}}}\right)\right] \text{ such that}$$

$$\mathcal{V}^\dagger_i[f_{\text{pad}}] \circ \zeta^{\text{out}}_{i,\text{pad}}(N^\alpha) = f'_{\text{pad}} \circ \zeta^{\text{out}}_{i,\text{pad}}(N^\alpha) \,. \tag{C.37}$$

H6 means that, for a branch N^α in a green layer, provided that one is in the subspace in which branch N^α happens, $\mathcal{S}_{\text{pad}}[(V_{N,i})_N]$'s causal structure only has the *strict* past of N^α signalling to N^α_{in}. This will be important to ensure that, when N^α is 'refilled', the action of any ζ^{out}_i's on it becomes an action on its strict past.

Induction Hypothesis 7 (H7)**.** *For a branch N^α in a red layer, we have*

$$\forall f \in \text{Lin}[\mathcal{H}_{N^\alpha_{\text{out}}}], \exists f' \in \text{Lin}\left[\mathcal{H}_F \otimes \left(\bigotimes_{O^\gamma \in \mathcal{F}^{\text{str}}_i(N^\alpha)} \mathcal{H}_{O^\gamma_{\text{in}}}\right)\right] \text{ such that}$$

$$\mathcal{V}_i[f_{\text{pad}}] \circ \zeta^{\text{in}}_{i,\text{pad}}(N^\alpha) = f'_{\text{pad}} \circ \zeta^{\text{in}}_{i,\text{pad}}(N^\alpha) \,. \tag{C.38}$$

H7 plays the same role as H6 in the reverse time direction.

Proof of the base case

H1 The proof that $\mathcal{S}_{\text{pad}}[(\text{EXCH}_N)_N]$ is unitary will rely on the lemmas of Section C.2.4. To use them, we will first introduce a way to show how bifurcation choices are enforced through the use of the EXCH's. For every A in Arr_Γ, we define $\text{WITNESS}_A :$ $\mathcal{H}_A \to \mathcal{H}_A \otimes \mathbb{C}^{|\text{Ind}_A|}$ by

$$\text{WITNESS}_A := \sum_{k_A \in \text{Ind}_A} \pi^{k_A}_A \otimes |k_A\rangle \,, \tag{C.39}$$

where the $\pi^{k_A}_A$'s are the projectors on the different sectors of A, and we've introduced an arbitrary basis of $\mathbb{C}^{|\text{Ind}_A|}$ labelled by A's index values. The point of WITNESS_A is simply to channel out the information about each arrow's index value.

For a given N, with respect to the sectorisations of the $\mathcal{H}_{N^\alpha_{\text{out}}}$, of the $\mathcal{H}_A$'s for the A's in $\text{in}(N)$ and $\text{out}(N)$, and to the sectorisation of the $\mathbb{C}^{|\text{Ind}_A|}$'s given by the previous basis, λ^{sec}_N is a route for $\left(\bigotimes_{A \in \text{out}(N)} \text{WITNESS}_A\right)_{\text{pad}} \circ \text{EXCH}_N$. Thus (because the compatibility with routes is preserved by the dagger compact structure [1]), $\mathcal{S}^{\textbf{Rel}}_{\text{pad}}[(\lambda^{\text{sec}}_N)_N] = \Lambda^{\text{sec}}_\Gamma$ is a route for $\mathcal{S}_{\text{pad}}\left[\left(\left(\bigotimes_{A \in \text{out}(N)} \text{WITNESS}_A\right)_{\text{pad}} \circ \text{EXCH}_N\right)_N\right]$. Therefore,

$$\mathcal{S}_{\text{pad}}\left[\left(\left(\bigotimes_{A\in\text{out}(N)}\text{WITNESS}_A\right)_{\text{pad}}\circ\text{EXCH}_N\right)_N\right]$$

$$=\sum_{\vec{k}\in\times_A\text{Ind}_A}\left(\bigotimes_A|k_A\rangle\langle k_A|\right)_{\text{pad}}\circ\mathcal{S}_{\text{pad}}\left[\left(\left(\bigotimes_{A\in\text{out}(N)}\text{WITNESS}_A\right)_{\text{pad}}\circ\text{EXCH}_N\right)_N\right]$$

$$\circ\left(\sum_{\vec{q}\in(\Lambda^{\text{sec}})^{-1}(\vec{k})}\bigotimes_{N^\alpha\in\text{Bran}_\Gamma}\pi_{N_{\text{out}}^\alpha}^{q_{N^\alpha}}\right)_{\text{pad}}$$

$$\overset{\text{Lemma C.2.4}}{=}\sum_{\vec{k}\in\text{PossVal}_\Gamma}\left(\bigotimes_A|k_A\rangle\langle k_A|\right)_{\text{pad}}\circ\mathcal{S}_{\text{pad}}\left[\left(\left(\bigotimes_{A\in\text{out}(N)}\text{WITNESS}_A\right)_{\text{pad}}\circ\text{EXCH}_N\right)_N\right]$$

$$\circ\left(\sum_{\vec{q}\in(\Lambda^{\text{sec}})^{-1}(\vec{k})}\bigotimes_{N^\alpha\in\text{Bran}_\Gamma}\pi_{N_{\text{out}}^\alpha}^{q_{N^\alpha}}\right)_{\text{pad}}$$

$$\overset{\text{Lemma C.2.3}}{=}\sum_{\vec{k}\in\text{PossVal}_\Gamma}\left(\bigotimes_A|k_A\rangle\langle k_A|\right)_{\text{pad}}\circ\mathcal{S}_{\text{pad}}\left[\left(\left(\bigotimes_{A\in\text{out}(N)}\text{WITNESS}_A\right)_{\text{pad}}\circ\text{EXCH}_N\right)_N\right]$$

$$\circ\left(\bigotimes_{N\in\text{Nodes}_\Gamma}\pi_{N_{\text{out}}^{\mu_N(\vec{k})}}^{(k_A)_{A\in\text{out}(N)}}\right)_{\text{pad}},$$

$$(\text{C.40})$$

where $\pi_{N_{\text{out}}^{\mu_N(\vec{k})}}^{(k_A)_{A\in\text{out}(N)}}$ is the projector on $\mathcal{H}_{N_{\text{out}}^{\mu_N(\vec{k})}}$'s sector labelled by $(k_A)_{A\in\text{out}(N)}$ (remember that for a given N^α, we have $\mathcal{H}_{N_{\text{out}}^\alpha}=\bigoplus_{(k_A)_{A\in\text{out}(N)}\in\text{Ind}_{N^\alpha}^{\text{out}}}\bigotimes_{A\in\text{out}(N)}\mathcal{H}_A^{k_A}$).

Moreover, we have $\left(\sum_{k\in\text{Ind}_A}\langle k|\right)_{\text{pad}}\circ\text{WITNESS}_A=\mathbb{1}_A$, so

$$\mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]$$

$$= \mathcal{S}_{\text{pad}}\left[\left(\left(\sum_{(k_A)_A \in \text{Ind}_N^{\text{out}}} \left(\bigotimes_{A \in \text{out}(N)} \langle k_A| \circ \text{WITNESS}_A\right)_{\text{pad}} \text{EXCH}_N\right)_N\right]$$

$$= \sum_{\vec{k} \in \times_A \text{Ind}_A} \left(\bigotimes_A \langle k_A|\right)_{\text{pad}} \mathcal{S}_{\text{pad}}\left[\left((\text{WITNESS}_A)_{\text{pad}} \circ \text{EXCH}_N\right)_N\right]$$

$$\overset{(\text{C.40})}{=} \sum_{\vec{k} \in \text{PossVal}_\Gamma} \left(\bigotimes_A \langle k_A|\right)_{\text{pad}} \circ \mathcal{S}_{\text{pad}}\left[\left(\left(\bigotimes_{A \in \text{out}(N)} \text{WITNESS}_A\right)_{\text{pad}} \circ \text{EXCH}_N\right)_N\right]$$

$$\circ \left(\bigotimes_{N \in \text{Nodes}_\Gamma} \pi^{(k_A)_{A \in \text{out}(N)}}_{N_{\text{out}}^{\mu_N(\vec{k})}}\right)_{\text{pad}}$$

$$= \sum_{\vec{k} \in \text{PossVal}_\Gamma} \mathcal{S}_{\text{pad}}\left[\left(\left(\bigotimes_{A \in \text{out}(N)} \pi_A^{k_A}\right)_{\text{pad}} \circ \text{EXCH}_N\right)_N\right] \circ \left(\bigotimes_{N \in \text{Nodes}_\Gamma} \pi^{(k_A)_{A \in \text{out}(N)}}_{N_{\text{out}}^{\mu_N(\vec{k})}}\right)_{\text{pad}}.$$

$$(\text{C.41})$$

A symmetric argument relying on $\Gamma^\top$ leads to

$$\mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]$$

$$= \sum_{\vec{k} \in \text{PossVal}_\Gamma} \left(\bigotimes_{N \in \text{Nodes}_\Gamma} \pi^{(k_A)_{A \in \text{in}(N)}}_{N_{\text{in}}^{\mu_N(\vec{k})}}\right)_{\text{pad}} \circ \mathcal{S}_{\text{pad}}\left[\left(\text{EXCH}_N \circ \left(\otimes_{A \in \text{in}(N)} \pi_A^{k_A}\right)_{\text{pad}}\right)_N\right].$$

$$(\text{C.42})$$

Furthermore, the projectors $\left(\otimes_{N \in \text{Nodes}_\Gamma} \pi^{(k_A)_{A \in \text{out}(N)}}_{N_{\text{out}}^{\mu_N(\vec{k})}}\right)_{\text{pad}}$, for $\vec{k} \in \text{PossVal}_\Gamma$, form a sectorisation of the input space of $\mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]$. Indeed, by Lemma C.2.3, the

$$\left(\underset{N}{\times} \{(k_A)_{A \in \text{out}(N)}\}_{\text{Ind}_{N^{\mu_N(\vec{k})}}^{\text{out}}}\right) \times \left(\underset{N^\alpha | \alpha \neq \mu_N(\vec{k})}{\times} \text{Ind}_{N^\alpha}^{\text{out}}\right) \qquad (\text{C.43})$$

are the preimage sets of the injective function $\Lambda_\Gamma^{\text{sec}}$, and therefore form a partition of its domain $\times_{N^\alpha} \text{Ind}_{N^\alpha}^{\text{out}}$. The sectorisation is thus obtained as a coarse-graining of that given by the $\otimes_{N^\alpha} \pi^{(k_A)_{A \in \text{out}(N)}}_{N_{\text{out}}^\alpha}$. Symmetrically, the $\left(\otimes_{N \in \text{Nodes}_\Gamma} \pi^{(k_A)_{A \in \text{in}(N)}}_{N_{\text{in}}^{\mu_N(\vec{k})}}\right)_{\text{pad}}$ form a sectorisation of $\mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]$'s codomain. Crucially, $\mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]$ is block diagonal with respect to these two sectorisations: indeed, for a given $\vec{k}$,

$$
\mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right] \circ \left(\bigotimes_{N\in\text{Nodes}_\Gamma} \pi_{N_{\text{out}}^{\mu_N(\vec{k})}}^{(k_A)_{A\in\text{out}(N)}}\right)_{\text{pad}}
$$

$$
\overset{\text{(C.41)}}{=} \mathcal{S}_{\text{pad}}\left[\left(\left(\bigotimes_{A\in\text{out}(N)} \pi_A^{k_A}\right)_{\text{pad}} \circ \text{EXCH}_N\right)_N\right]
$$

$$
\overset{\text{(C.17)}}{=} \mathcal{S}_{\text{pad}}\left[\left(\text{EXCH}_N \circ \left(\bigotimes_{A\in\text{in}(N)} \pi_A^{k_A}\right)_{\text{pad}}\right)_N\right]
$$

$$
\overset{\text{(C.42)}}{=} \left(\bigotimes_{N\in\text{Nodes}_\Gamma} \pi_{N_{\text{in}}^{\mu_N(\vec{k})}}^{(k_A)_{A\in\text{in}(N)}}\right)_{\text{pad}} \circ \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right].
$$

(C.44)

All that is left for us to prove is that all of these blocks, which we will denote as $T^{\vec{k}}$'s, are unitary (with respect to the suitable restrictions of their domain and codomain). We start by computing

$$
T^{\vec{k}} = \mathcal{S}_{\text{pad}}\left[\left(\left(\bigotimes_{A\in\text{out}(N)} \pi_A^{k_A}\right)_{\text{pad}} \circ \text{EXCH}_N\right)_N\right]
$$

$$
\overset{\text{(C.20)}}{=} \mathcal{S}_{\text{pad}}\left[\left(\left(\bigotimes_{A\in\text{out}(N)} \pi_A^{k_A}\right)_{\text{pad}} \circ i_{N,\text{pad}}^{\mu_N(\vec{k})} \circ \left(\text{SWAP}_{N_{\text{in}}^{\mu_N(\vec{k})},N_{\text{out}}^{\mu_N(\vec{k})}} \otimes \left(\bigotimes_{\beta\neq\mu_N(\vec{k})} \Theta_{N^\beta}\right)\right) \circ p_{N,\text{pad}}^{\mu_N(\vec{k})}\right)_N\right]
$$

$$
\overset{\text{(C.17)}}{=} \text{Tr}_{A\in\text{Arr}_\Gamma^{\text{int}}}\left[\bigotimes_N \left(\left(\bigotimes_{A\in\text{out}(N)} \pi_A^{k_A}\right)_{\text{pad}} \circ i_{N,\text{pad}}^{\mu_N(\vec{k})} \circ \text{SWAP}_{N_{\text{in}}^{\mu_N(\vec{k})},N_{\text{out}}^{\mu_N(\vec{k})}} \circ p_{N,\text{pad}}^{\mu_N(\vec{k})}\right) \otimes \left(\bigotimes_{M,\beta\neq\mu_M(\vec{k})} \Theta_{M^\beta}\right)\right]
$$

$$
= \left(\left(\bigotimes_N p_N^{\mu_N(\vec{k})}\right) \circ \left(\bigotimes_{A\in\text{Arr}_\Gamma} \pi_A^{k_A}\right) \circ \left(\bigotimes_N i_N^{\mu_N(\vec{k})}\right)\right) \otimes \left(\bigotimes_{M,\beta\neq\mu_M(\vec{k})} \Theta_{M^\beta}\right).
$$

(C.45)

Remember that $i_N^{\mu_N(\vec{k})}$ is the injection $\mathcal{H}_{N^{\mu_N(\vec{k})}}^{\text{out}} \to \mathcal{H}_N^{\text{out}} = \bigotimes_{A\in\text{out}(N)} \mathcal{H}_A$, and $p_N^{\mu_N(\vec{k})}$ is the projection $\mathcal{H}_N^{\text{in}} = \bigotimes_{A\in\text{in}(N)} \mathcal{H}_A \to \mathcal{H}_{N^{\mu_N(\vec{k})}}^{\text{in}}$. We will also define the injection $i_N^{(k_A)_{A\in\text{out}(N)}} : \bigotimes_{A\in\text{out}(N)} \mathcal{H}_A^{k_A} \to \mathcal{H}_{N^{\mu_N(\vec{k})}}^{\text{out}}$, and the projection $p_N^{(k_A)_{A\in\text{in}(N)}} : \mathcal{H}_{N^{\mu_N(\vec{k})}}^{\text{in}} \to \bigotimes_{A\in\text{in}(N)} \mathcal{H}_A^{k_A}$: these map $T^{\vec{k}}$'s to the suitable domains and codomains. Note that we then have

$$
\bigotimes_N i_N^{\mu_N(\vec{k})} \circ i_N^{(k_A)_{A\in\text{out}(N)}} = \bigotimes_A i_A^{k_A},
$$

(C.46a)

$$
\bigotimes_N p_N^{(k_A)_{A\in\text{out}(N)}} \circ p_N^{\mu_N(\vec{k})} = \bigotimes_A p_A^{k_A},
$$

(C.46b)

where $i_A^{k_A}$ is the injection $\mathcal{H}_A^{k_A} \to \mathcal{H}_A$ and $p_A^{k_A}$ is the projection $\mathcal{H}_A \to \mathcal{H}_A^{k_A}$. Thus,

$$
\begin{aligned}
&\left(\bigotimes_N p_N^{(k_A)_{A \in \text{in}(N)}} \right)_{\text{pad}} \circ T^{\vec{k}} \circ \left(\bigotimes_N i_N^{(k_A)_{A \in \text{out}(N)}} \right)_{\text{pad}} \\
&= \left(\bigotimes_A p_A^{k_A} \circ \pi_A^{k_A} \circ i_A^{k_A} \right) \otimes \left(\bigotimes_{M, \beta \neq \mu_M(\vec{k})} \Theta_{M^\beta} \right) \\
&= \left(\bigotimes_A \mathbb{1}_{A^{k_A}} \right) \otimes \left(\bigotimes_{M, \beta \neq \mu_M(\vec{k})} \Theta_{M^\beta} \right) .
\end{aligned} \tag{C.47}
$$

Each of the blocks composing $\mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]$ is thus unitary once restricted to the suitable subspaces, so $\mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]$ is unitary as well.

H2   We define, for all branches N^α,

$$
Z^{\text{out}}(N^\alpha) := \Lambda_\Gamma^{-1} \left(\{1\}_{\text{Happens}_{N^\alpha}} \times \underset{M^\beta \neq N^\alpha}{\bigtimes} \text{Happens}_{M^\beta} \right), \tag{C.48a}
$$

$$
\zeta^{\text{out}}(N^\alpha) := \sum_{(l_{M^\beta})_{M^\beta \in \text{Bran}_\Gamma} \in Z^{\text{out}}(N^\alpha)} \left(\bigotimes_{M^\beta} \pi_{M_{\text{out}}^\beta}^{l_{M^\beta}} \right), \tag{C.48b}
$$

and similarly for the Z^{in}'s and ζ^{in}'s. Note that

$$
Z^{\text{out}}(N^\alpha) = \bigsqcup_{\substack{\vec{k} \in \text{PossVal}_\Gamma \\ \mu_N(\vec{k}) = \alpha}} (\Lambda_\Gamma^{\text{sec}})^{-1}\left(\vec{k} \right). \tag{C.49}
$$

Given their definition, the ζ^{out}'s are commuting orthogonal projectors. Furthermore, as green dashed arrows in Γ^{Bran} represent Λ_Γ's causal structure, we have, for any branch N^α,

$$
Z^{\text{out}}(N^\alpha) := \tilde{Z}^{\text{out}}(N^\alpha) \times \left(\underset{\exists \text{ no green dashed arrow } M^\beta \to N^\alpha}{\bigtimes} \text{Ind}_{M^\beta}^{\text{out}} \right) \tag{C.50}
$$

Through (C.48b), this implies that $\zeta^{\text{out}}(N^\alpha)$ acts trivially on the M^β's that are not linked to N^α by a green dashed arrow. We can thus in particular see it as the padding of an operator acting only on $\mathcal{P}(N^\alpha)$, or on $\mathcal{P}^{\text{str}}(N^\alpha)$ if N^α is in a red layer. The same applies symmetrically for the ζ^{in}'s. Finally, (C.44) implies

$$\mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right] \circ \zeta^{\text{out}}(N^\alpha) = \sum_{\substack{\vec{k} \in \text{PossVal}_\Gamma \\ \mu_N(\vec{k}) = \alpha}} \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right] \circ \left(\bigotimes_{N \in \text{Nodes}_\Gamma} \pi_{N_{\text{out}}^{\mu_N(\vec{k})}}^{(k_A)_{A \in \text{out}(N)}}\right)_{\text{pad}}$$

$$= \sum_{\substack{\vec{k} \in \text{PossVal}_\Gamma \\ \mu_N(\vec{k}) = \alpha}} \left(\bigotimes_{N \in \text{Nodes}_\Gamma} \pi_{N_{\text{out}}^{\mu_N(\vec{k})}}^{(k_A)_{A \in \text{out}(N)}}\right)_{\text{pad}} \circ \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]$$

$$= \zeta^{\text{in}}(N^\alpha) \circ \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right] ;$$

$$(\text{C.51})$$

thus, $\mathcal{V}_0[\zeta^{\text{out}}(N^\alpha)] = \zeta^{\text{in}}(N^\alpha)$.

H3   We will prove that $Z^{\text{out}}(N^\alpha) \cap \bar{Z}^{\text{out}}(M^\beta)$ is of the form $\tilde{Z} \times \text{Ind}_{M^\beta}^{\text{out}}$, from which (H3) derives. This set can be computed, using bra-ket notations in **Rel**, as $\left(\langle 1|_{\text{Happens}_{N^\alpha}} \otimes \langle 0|_{\text{Happens}_{M^\beta}}\right)_{\text{pad}} \circ \Lambda_\Gamma$. Yet, one can see from the definition of the λ^{aug}'s that

$$\langle 0|_{\text{Happens}_{M^\beta},\text{pad}} \circ \lambda_M^{\text{aug}} = \langle 0|_{\text{Happens}_{M^\beta},\text{pad}} \circ \lambda_M^{\text{aug}} \circ |\text{Ind}_{M^\beta}^{\text{out}}\rangle\langle\text{Ind}_{M^\beta}^{\text{out}}|_{\text{Ind}_{M^\beta}^{\text{out}},\text{pad}} ; \quad (\text{C.52})$$

thus,

$$\left(\langle 1|_{\text{Happens}_{N^\alpha}} \otimes \langle 0|_{\text{Happens}_{M^\beta}}\right)_{\text{pad}} \circ \Lambda_\Gamma$$

$$= \left(\langle 1|_{\text{Happens}_{N^\alpha}} \otimes \langle 0|_{\text{Happens}_{M^\beta}}\right)_{\text{pad}} \circ \mathcal{S}_\Gamma^{\textbf{Rel}}\left[(\lambda_N^{\text{aug}})_N\right]$$

$$= \left(\langle 1|_{\text{Happens}_{N^\alpha}} \otimes \langle 0|_{\text{Happens}_{M^\beta}}\right)_{\text{pad}} \circ \mathcal{S}_\Gamma^{\textbf{Rel}}\left[(\lambda_N^{\text{aug}})_{N \neq M} \times \left(\lambda_M^{\text{aug}} \circ |\text{Ind}_{M^\beta}^{\text{out}}\rangle\langle\text{Ind}_{M^\beta}^{\text{out}}|_{\text{Ind}_{M^\beta}^{\text{out}},\text{pad}}\right)\right]$$

$$= \left(\left(\langle 1|_{\text{Happens}_{N^\alpha}} \otimes \langle 0|_{\text{Happens}_{M^\beta}}\right)_{\text{pad}} \circ \mathcal{S}_\Gamma^{\textbf{Rel}}\left[(\lambda_N^{\text{aug}})_N\right] \circ |\text{Ind}_{M^\beta}^{\text{out}}\rangle_{\text{Ind}_{M^\beta}^{\text{out}}}\right) \otimes \langle\text{Ind}_{M^\beta}^{\text{out}}|_{\text{Ind}_{M^\beta}^{\text{out}}} ,$$

$$(\text{C.53})$$

which shows that indeed $Z^{\text{out}}(N^\alpha) \cap \bar{Z}^{\text{out}}(M^\beta) = \tilde{Z} \times \text{Ind}_{M^\beta}^{\text{out}}$. The proof for the Z^{in}'s is symmetric.

H4   (H4) comes from the fact that, for $\alpha \neq \beta$, one has $Z^{\text{out}}(N^\alpha) \cap Z^{\text{out}}(N^\beta) = \varnothing$, which can be derived directly from (C.49).

H5   We take $Q = \{N^{\alpha(N)} \mid N \in \tilde{Q}\} \subseteq \text{Bran}_\Gamma$. Then,

$$\mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right] \circ \prod_{N \in \tilde{Q}} \zeta^{\text{out}}(N^{\alpha(N)})$$

$$\overset{(C.49)}{=} \sum_{\substack{\vec{k} \in \text{PossVal}_\Gamma \\ \forall N \in \tilde{Q}, \mu_N(\vec{k}) = \alpha(N)}} \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right] \circ \left(\bigotimes_{N \in \text{Nodes}_\Gamma} \pi_{N_{\text{out}}^{\mu_N(\vec{k})}}^{(k_A)_{A \in \text{out}(N)}}\right)_{\text{pad}}$$

$$\overset{(C.41)}{=} \sum_{\substack{\vec{k} \in \text{PossVal}_\Gamma \\ \forall N \in \tilde{Q}, \mu_N(\vec{k}) = \alpha(N)}} \mathcal{S}_{\text{pad}}\left[\left(\left(\bigotimes_{A \in \text{out}(N)} \pi_A^{k_A}\right)_{\text{pad}} \circ \text{EXCH}_N\right)_N\right]$$

$$= \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_{N \notin \tilde{Q}} \times \left(\sum_{(k_A)_{A \in \text{out}(N)} \in \text{Ind}_{N^\alpha}^{\text{out}}} \left(\bigotimes_{A \in \text{out}(N)} \pi_A^{k_A}\right)_{\text{pad}} \circ \text{EXCH}_N\right)_{N \in \tilde{Q}}\right]$$

$$= \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_{N \notin \tilde{Q}} \times (\pi_{N^{\text{out}}}^\alpha \circ \text{EXCH}_N)_{N \in \tilde{Q}}\right]$$

$$\overset{(C.20)}{=} \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_{N \notin \tilde{Q}} \times \left(V_{0,N}^\alpha\right)_{N \in \tilde{Q}}\right].$$

$$(C.54)$$

H6 We take N^α in a green layer, and $f \in \text{Lin}\left[\mathcal{H}_{N_{\text{in}}^\alpha}\right]$. We then have (note that $\zeta^{\text{in}}(N^\alpha)$ doesn't act on N_{in}^α)

$$\mathcal{V}_0^\dagger\left[f_{\text{pad}}\right] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha) = \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]^\dagger \circ f_{\text{pad}} \circ \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha)$$

$$\overset{(C.51)}{=} \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]^\dagger \circ f_{\text{pad}} \circ \zeta_{\text{pad}}^{\text{in}}(N^\alpha) \circ \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha)$$

$$= \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]^\dagger \circ \zeta_{\text{pad}}^{\text{in}}(N^\alpha) \circ f_{\text{pad}} \circ \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha)$$

$$\overset{(C.51)}{=} \zeta_{\text{pad}}^{\text{out}}(N^\alpha) \circ \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right]^\dagger \circ f_{\text{pad}} \circ \mathcal{S}_{\text{pad}}\left[(\text{EXCH}_N)_N\right] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha)$$

$$\overset{(C.48b),(C.49)}{=} \sum_{\substack{\vec{k},\vec{l} \in \text{PossVal}_\Gamma \\ \mu_N(\vec{k}) = \mu_N(\vec{l}) = \alpha}} \left(T^{\vec{l}}\right)^\dagger \circ f_{\text{pad}} \circ T^{\vec{k}}.$$

$$(C.55)$$

Furthermore, taking $M^\beta \notin \mathcal{P}^{\text{str}}(N^\alpha)$, because N^α is in a green layer we know that there is no red dashed arrow from M^β to N^α, and thus $\zeta^{\text{in}}(M^\beta)$ doesn't act on N_{in}^α. We can thus apply the same computation to it as well, which leads to

$$
\begin{aligned}
\mathcal{V}_0^\dagger \left[f_{\text{pad}} \right] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha) &= \mathcal{V}_0 \left[f_{\text{pad}} \right] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha) \circ \left(\zeta_{\text{pad}}^{\text{out}}(M^\beta) + \bar{\zeta}_{\text{pad}}^{\text{out}}(M^\beta) \right) \\
&= \zeta_{\text{pad}}^{\text{out}}(N^\alpha) \circ \zeta_{\text{pad}}^{\text{out}}(M^\beta) \circ \mathcal{V}_0 \left[f_{\text{pad}} \right] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha) \circ \zeta_{\text{pad}}^{\text{out}}(M^\beta) \\
&+ \zeta_{\text{pad}}^{\text{out}}(N^\alpha) \circ \bar{\zeta}_{\text{pad}}^{\text{out}}(M^\beta) \circ \mathcal{V}_0 \left[f_{\text{pad}} \right] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha) \circ \bar{\zeta}_{\text{pad}}^{\text{out}}(M^\beta) \\
&= \sum_{\substack{ \vec{k}, \vec{l} \in \text{PossVal}_\Gamma \\ \mu_N(\vec{k}) = \mu_N(\vec{l}) = \alpha \\ \mu_M(\vec{k}) = \beta \iff \mu_M(\vec{l}) = \beta }} \left(T^{\vec{l}} \right)^\dagger \circ f_{\text{pad}} \circ T^{\vec{k}} ;
\end{aligned}
\tag{C.56}
$$

in other words, in the sum above, the values of $\vec{k}$ and $\vec{l}$ that lead to attributing different statuses to M^β correspond to null terms, so that one can skip them in the summation. More generally, one can apply this reasoning to all branches $M^\beta \notin \mathcal{P}^{\text{str}}(N^\alpha)$, leading to

$$
\mathcal{V}_0 \left[f_{\text{pad}} \right] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha) = \sum_{\substack{ \vec{k}, \vec{l} \in \text{PossVal}_\Gamma \\ \mu_N(\vec{k}) = \mu_N(\vec{l}) = \alpha \\ \forall M^\beta \notin \mathcal{P}^{\text{str}}(N^\alpha), \mu_M(\vec{k}) = \beta \iff \mu_M(\vec{l}) = \beta }} \left(T^{\vec{l}} \right)^\dagger \circ f_{\text{pad}} \circ T^{\vec{k}}.
\tag{C.57}
$$

Using (C.47), we rewrite $T^{\vec{k}}$, for an arbitrary $\vec{k}$, as

$$
\begin{aligned}
T^{\vec{k}} &= \left(\bigotimes_M p_M^{(k_A)_{A \in \text{in}(M)}} \right)_{\text{pad}}^\dagger \circ \left(\left(\bigotimes_A \mathbb{1}_{A^{k_A}} \right) \otimes \left(\bigotimes_{M, \beta \neq \mu_M(\vec{k})} \Theta_{M^\beta} \right) \right) \\
&\circ \left(\bigotimes_M i_M^{(k_A)_{A \in \text{out}(M)}} \right)_{\text{pad}}^\dagger .
\end{aligned}
\tag{C.58}
$$

Now, we take $\vec{k}, \vec{l} \in \text{PossVal}_\Gamma$ satisfying the requirements we pinned down earlier; we can then compute

$$T^{\vec{l}^\dagger} \circ f_{\text{pad}} \circ T^{\vec{k}}$$

$$= \left(\bigotimes_M i_M^{(l_A)_{A\in\text{out}(M)}} \right)_{\text{pad}} \circ \left(\left(\bigotimes_A \mathbb{1}_{A^{l_A}} \right) \otimes \left(\bigotimes_{M,\beta\neq\mu_M(\vec{l})} \Theta_{M^\beta}^\dagger \right) \right)$$

$$\circ \left(\bigotimes_M p_M^{(l_A)_{A\in\text{in}(M)}} \right)_{\text{pad}} \circ f_{\text{pad}} \circ \left(\bigotimes_M p_M^{(k_A)_{A\in\text{in}(M)}} \right)_{\text{pad}}^\dagger$$

$$\circ \left(\left(\bigotimes_A \mathbb{1}_{A^{k_A}} \right) \otimes \left(\bigotimes_{M,\beta\neq\mu_M(\vec{k})} \Theta_{M^\beta} \right) \right) \circ \left(\bigotimes_M i_M^{(k_A)_{A\in\text{out}(M)}} \right)_{\text{pad}}^\dagger$$

$$= \left(\bigotimes_M i_M^{(l_A)_{A\in\text{out}(M)}} \right)_{\text{pad}} \circ \left[\left(p_N^{(l_A)_{A\in\text{in}(N)}} \circ f \circ \left(p_N^{(k_A)_{A\in\text{in}(N)}} \right)^\dagger \right) \right. \tag{C.59}$$

$$\otimes \left(\bigotimes_{\substack{M\neq N \\ \mu_M(\vec{l})\neq\mu_M(\vec{k})}} \left(\Theta_{M^{\mu_M(\vec{k})}}^\dagger \circ \left(p_M^{(k_A)_{A\in\text{in}(M)}} \right)^\dagger \right) \otimes \left(p_M^{(l_A)_{A\in\text{in}(M)}} \circ \Theta_{M^{\mu_M(\vec{l})}} \right) \right)$$

$$\otimes \left(\bigotimes_{\substack{M\neq N \\ \mu_M(\vec{l})=\mu_M(\vec{k})=1}} p_M^{(l_A)_{A\in\text{in}(M)}} \circ \left(p_M^{(k_A)_{A\in\text{in}(M)}} \right)^\dagger \right) \left. \right]_{\text{pad}} \circ \left(\bigotimes_M i_M^{(k_A)_{A\in\text{out}(M)}} \right)_{\text{pad}}^\dagger .$$

Note that each of the $p_M^{(l_A)_{A\in\text{in}(M)}} \circ \left(p_M^{(k_A)_{A\in\text{in}(M)}} \right)^\dagger$ terms, for M such that $M^{\mu_M(\vec{k})} \notin \mathcal{P}^{\text{str}}(N^\alpha) \cup \{N^\alpha\}$, can be rewritten as $\bigotimes_{A\in\text{in}(M)} p_A^{l_A} \circ i_A^{k_A}$ (which is the identity if $k_A = l_A \forall A \in \text{in}(M)$, and zero otherwise).

Now, for any M such that $M^{\mu_M(\vec{k})} \notin \mathcal{P}^{\text{str}}(N^\alpha)$, and for any O such that $O^{\mu_O(\vec{k})} \in \mathcal{P}^{\text{str}}(N^\alpha) \cup \{N^\alpha\}$, there is no arrow $A \in \text{Link}(M,O)$ such that $|A^{k_A}| \neq 1$, as that would imply the existence of a solid arrow from $M^{\mu_M(\vec{k})}$ to $O^{\mu_O(\vec{k})}$, which would contradict $M^{\mu_M(\vec{k})} \notin \mathcal{P}^{\text{str}}(N^\alpha)$. Thus, all of the non-trivial arrows in $\text{out}(M)$ go to O's such that $O \neq N$ and $\mu_O(\vec{l}) = \mu_O(\vec{k})$. Thus this implies that, if one doesn't have $k_A = l_A \forall A \in \text{out}(M)$ then the whole expression is null; while otherwise, the term in square brackets acts trivially on each of the $A \in \text{out}(M)$ – in other words, the arrows coming out of M are never acted on and simply link $i_M^{(k_A)_{A\in\text{out}(M)}\dagger}$ directly to $i_M^{(l_A)_{A\in\text{out}(M)}}$. One can thus reorganise this expression (neglecting the existence of all the trivial spaces) as

$$
T^{\vec{l}\,\dagger} \circ f_{\text{pad}} \circ T^{\vec{k}} = \left[\left(\bigotimes_{\substack{M \\ M^{\mu_M(\vec{l})} \in \mathcal{P}^{\text{str}}(N^\alpha)}} i_M^{(l_A)_{A\in\text{out}(M)}}\right) \circ \left[\left(p_N^{(l_A)_{A\in\text{in}(N)}} \circ f \circ \left(p_N^{(k_A)_{A\in\text{in}(N)}}\right)^\dagger\right)\right.\right.
$$

$$
\otimes \left(\bigotimes_{\substack{M \\ M^{\mu_M(\vec{l})},M^{\mu_M(\vec{k})} \in \mathcal{P}^{\text{str}}(N^\alpha) \\ \mu_M(\vec{l}) \neq \mu_M(\vec{k})}} \left(\Theta_{M^{\mu_M(\vec{k})}}^\dagger \circ \left(p_M^{(k_A)_{A\in\text{in}(M)}}\right)^\dagger\right) \otimes \left(p_M^{(l_A)_{A\in\text{in}(M)}} \circ \Theta_{M^{\mu_M(\vec{l})}}\right)\right)
$$

$$
\left.\otimes \left(\bigotimes_{\substack{M \\ M^{\mu_M(\vec{l})},M^{\mu_M(\vec{k})} \in \mathcal{P}^{\text{str}}(N^\alpha) \\ \mu_M(\vec{l})=\mu_M(\vec{k})}} \bigotimes_{A\in\text{in}(M)} p_A^{l_A}\circ i_A^{k_A}\right) \otimes \left(\bigotimes_{\substack{O \\ O^{\mu_O(\vec{k})}\notin\mathcal{P}^{\text{str}}(N^\alpha)}} \bigotimes_{\substack{M \\ M^{\mu_M(\vec{k})}\in\mathcal{P}^{\text{str}}(N^\alpha)}} \bigotimes_{A\in\text{Link}(M,O)} p_A^{l_A}\circ i_A^{k_A}\right)\right]
$$

$$
\circ \left(\bigotimes_{\substack{M \\ M^{\mu_M(\vec{k})}\in\mathcal{P}^{\text{str}}(N^\alpha)}} i_M^{(k_A)_{A\in\text{out}(M)}}\right)^\dagger_{\text{pad}} \right]_{\text{pad}} \otimes \left(\left(\bigotimes_{\substack{M \\ M^{\mu_M(\vec{k})}\notin\mathcal{P}^{\text{str}}(N^\alpha)}} \pi_{M_{\text{out}}^{\mu_M(\vec{k})}}^{(k_A)_{A\in\text{out}(M)}}\right) \otimes \left(\bigotimes_{\substack{M,\beta\neq\mu_M(\vec{k}) \\ M^\beta\notin\mathcal{P}^{\text{str}}(N^\alpha)}} \mathbb{1}_{M_{\text{out}}^\beta}\right)\right) ;
$$

$$\tag{C.60}$$

note how the action on the M_{out}^β's for $M^\beta \notin \mathcal{P}^{\text{str}}(N^\alpha)$ now only consists of a projector independent of f. Note that in the second bracket of the third line, the condition $M^{\mu_M(\vec{k})} \in \mathcal{P}^{\text{str}}(N^\alpha)$ could equivalently have been replaced with $M^{\mu_M(\vec{l})} \in \mathcal{P}^{\text{str}}(N^\alpha)$, because we know that $M^{\mu_M(\vec{k})} \notin \mathcal{P}^{\text{str}}(N^\alpha) \implies M^{\mu_M(\vec{l})} = M^{\mu_M(\vec{k})} \notin \mathcal{P}^{\text{str}}(N^\alpha)$, and conversely; so that we have the equivalence $M^{\mu_M(\vec{k})} \notin \mathcal{P}^{\text{str}}(N^\alpha) \iff M^{\mu_M(\vec{l})} \notin \mathcal{P}^{\text{str}}(N^\alpha)$.

Both bracketed terms in the third line can be rewritten simply as Kronecker deltas, of the form:

$$
\left(\prod_{\substack{M \\ M^{\mu_M(\vec{l})},M^{\mu_M(\vec{k})}\notin\mathcal{P}^{\text{str}}(N^\alpha) \\ \mu_M(\vec{l})=\mu_M(\vec{k})}} \prod_{A\in\text{in}(M)} \delta_{k_A,l_A}\right) \cdot \left(\prod_{\substack{O \\ O^{\mu_O(\vec{k})}\notin\mathcal{P}^{\text{str}}(N^\alpha)}} \prod_{\substack{M \\ M^{\mu_M(\vec{k})}\in\mathcal{P}^{\text{str}}(N^\alpha)}} \prod_{A\in\text{Link}(M,O)} \delta_{k_A,l_A}\right) \cdot
$$

$$\tag{C.61}$$

We now take $\vec{q} = (q^{O^\gamma})_{O^\gamma\in\text{Bran}_\Gamma}, \vec{r} = (r^{O^\gamma})_{O^\gamma\in\text{Bran}_\Gamma} \in \bigtimes_{O^\gamma\in\text{Bran}_\Gamma} \text{Ind}_{O^\gamma}^{\text{out}}$. We then have

$$
\left(\bigotimes_{O^\gamma \in \mathbf{Bran}_\Gamma} \pi_{O^\gamma_{\text{out}}}^{r^{O^\gamma}} \right) \circ \mathcal{V}_0^\dagger[f_{\text{pad}}] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha) \circ \left(\bigotimes_{O^\gamma \in \mathbf{Bran}_\Gamma} \pi_{O^\gamma_{\text{out}}}^{q^{O^\gamma}} \right)
$$

$$
= \left(\bigotimes_{O^\gamma \in \mathbf{Bran}_\Gamma} \pi_{O^\gamma_{\text{out}}}^{r^{O^\gamma}} \right) \circ \mathcal{S}_{\text{pad}} \left[(\text{EXCH}_N)_N \right]^\dagger \circ f_{\text{pad}} \circ \mathcal{S}_{\text{pad}} \left[(\text{EXCH}_N)_N \right] \circ \left(\bigotimes_{O^\gamma \in \mathbf{Bran}_\Gamma} \pi_{O^\gamma_{\text{out}}}^{q^{O^\gamma}} \right) \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha)
$$

$$
= \left(\bigotimes_{O^\gamma \in \mathbf{Bran}_\Gamma} \pi_{O^\gamma_{\text{out}}}^{r^{O^\gamma}} \right) \circ \left(T^{\Lambda_\Gamma^{\text{sec}}(\vec{r})} \right)^\dagger \circ f_{\text{pad}} \circ T^{\Lambda_\Gamma^{\text{sec}}(\vec{q})} \circ \left(\bigotimes_{O^\gamma \in \mathbf{Bran}_\Gamma} \pi_{O^\gamma_{\text{out}}}^{q^{O^\gamma}} \right) \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha).
$$

$$\tag{C.62}$$

Note that $\mu_M \circ \Lambda_\Gamma^{\text{sec}}(\vec{q})$ denotes the only branch β of M such that the M^β term of $\Lambda_\Gamma(\vec{q})$, which we denote $\Lambda_\Gamma^{M^\beta}(\vec{q})$, is 1. By the previous considerations, the term above can thus be non null only if $\Lambda_\Gamma^{N^\alpha}(\vec{q}) = \Lambda_\Gamma^{N^\alpha}(\vec{r}) = 1$ and if $\Lambda_\Gamma^{M^\beta}(\vec{q}) = \Lambda_\Gamma^{M^\beta}(\vec{r}) \,\forall M^\beta \notin \mathcal{P}^{\text{str}}(N^\alpha)$. Furthermore, when this is the case, then we can use (C.60) and get

$$
\left(\bigotimes_{O^\gamma \in \mathbf{Bran}_\Gamma} \pi_{O^\gamma_{\text{out}}}^{r^{O^\gamma}} \right) \circ \mathcal{V}_0^\dagger[f_{\text{pad}}] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha) \circ \left(\bigotimes_{O^\gamma \in \mathbf{Bran}_\Gamma} \pi_{O^\gamma_{\text{out}}}^{q^{O^\gamma}} \right)
$$

$$
= F^{(r^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)}, (q^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)}} \otimes \left(\bigotimes_{M^\beta \notin \mathcal{P}^{\text{str}}(N^\alpha)} \pi_{M^\beta_{\text{out}}}^{q^{M^\beta}} \right)
$$

$$\tag{C.63}$$

$$
\cdot \prod_{O^\gamma \notin \mathcal{P}^{\text{str}}(N^\alpha)} \delta_{q^{O^\gamma}, r^{O^\gamma}} \,,
$$

where

$$F^{(r^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\mathrm{str}}(N^\alpha)}, (q^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\mathrm{str}}(N^\alpha)}}$$

$$= \left(\bigotimes_{O^\gamma \in \mathcal{P}^{\mathrm{str}}(N^\alpha)} \pi^{r^{O^\gamma}}_{O_{\mathrm{out}}^\gamma} \right) \circ \left(\bigotimes_{\substack{M^\beta \in \mathcal{P}^{\mathrm{str}}(N^\alpha) \\ \Lambda_\Gamma^{M^\beta}(\vec{r})=1}} i_M^{(l_A)_{A \in \mathrm{out}(M)}} \right)_{\mathrm{pad}} \circ \left[\left(p_N^{(l_A)_{A \in \mathrm{in}(N)}} \circ f \circ \left(p_N^{(k_A)_{A \in \mathrm{in}(N)}} \right)^\dagger \right) \right.$$

$$\otimes \left. \left(\bigotimes_{\substack{M \text{ s.t. } \exists \beta, \beta': \\ M^\beta, M^{\beta'} \in \mathcal{P}^{\mathrm{str}}(N^\alpha) \\ \Lambda_\Gamma^{M^\beta}(\vec{q})=\Lambda_\Gamma^{M^{\beta'}}(\vec{r})=1}} \left(\Theta_{M^\beta}^\dagger \circ \left(p_M^{(k_A)_{A \in \mathrm{in}(M)}} \right)^\dagger \right) \otimes \left(p_M^{(l_A)_{A \in \mathrm{in}(M)}} \circ \Theta_{M^{\beta'}} \right) \right) \right]$$

$$\circ \left(\bigotimes_{\substack{M^\beta \in \mathcal{P}^{\mathrm{str}}(N^\alpha) \\ \Lambda_\Gamma^{M^\beta}(\vec{q})=1}} i_M^{\cdot (k_A)_{A \in \mathrm{out}(M)}} \right)^\dagger_{\mathrm{pad}} \circ \left(\bigotimes_{O^\gamma \in \mathcal{P}^{\mathrm{str}}(N^\alpha)} \pi^{q^{O^\gamma}}_{O_{\mathrm{out}}^\gamma} \right) \cdot \left(\prod_{\substack{M^\beta \in \mathcal{P}^{\mathrm{str}}(N^\alpha) \\ \Lambda_\Gamma^{M^\beta}(\vec{r})=\Lambda_\Gamma^{M^\beta}(\vec{q})=1}} \prod_{A \in \mathrm{in}(M)} \delta_{k_A, l_A} \right)$$

$$\cdot \left(\prod_{\substack{O \\ \sum_{O^\gamma \in \mathcal{P}^{\mathrm{str}}(N^\alpha)} \Lambda_\Gamma^{O^\gamma}(\vec{q})=0}} \prod_{\substack{M \\ \sum_{M^\beta \in \mathcal{P}^{\mathrm{str}}(N^\alpha)} \Lambda_\Gamma^{M^\beta}(\vec{q})=1}} \prod_{A \in \mathtt{Link}(M,O)} \delta_{k_A, l_A} \right),$$

$$\tag{C.64}$$

with $\vec{k} := \Lambda_\Gamma^{\mathrm{sec}}(\vec{q})$, $\vec{l} := \Lambda_\Gamma^{\mathrm{sec}}(\vec{r})$. Note how $F^{(r^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\mathrm{str}}(N^\alpha)}, (q^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\mathrm{str}}(N^\alpha)}}$, which comes from the term in square brackets in (C.60) and acts only on P and on $\mathcal{P}^{\mathrm{str}}(N^\alpha)$, doesn't depend on the value of $(q^{O^\gamma})_{O^\gamma \notin \mathcal{P}^{\mathrm{str}}(N^\alpha)}$: indeed, the values of $\Lambda_\Gamma^{M^\beta}(\vec{q})$ and of $\Lambda_\Gamma^{M^\beta}(\vec{r})$ don't depend on the values of the q^{O^γ} for $O^\gamma \notin \mathcal{P}^{\mathrm{str}}(N^\alpha)$, as there are no green dashed arrows from these O^γ's to any $M^\beta \in \mathcal{P}^{\mathrm{str}}(N^\alpha)$. Similarly, the relevant values of the k_A's are those such that $A \in \mathrm{out}(M)$ for some $M^\beta \in \mathcal{P}^{\mathrm{str}}(N^\alpha)$ such that $\Lambda_\Gamma^{M^\beta}(\vec{q}) = 1$; thus they are just equal to the A-value of q^{M^β}. The same goes for the l_A's.

So far, we proved that (C.63) holds for $\vec{q}$ and $\vec{r}$ satisfying: $\Lambda_\Gamma^{N^\alpha}(\vec{q}) = \Lambda_\Gamma^{N^\alpha}(\vec{r}) = 1$ and $\Lambda_\Gamma^{M^\beta}(\vec{q}) = \Lambda_\Gamma^{M^\beta}(\vec{r}) \; \forall M^\beta \notin \mathcal{P}^{\mathrm{str}}(N^\alpha)$. We now want to prove that the same holds when the latter condition is not satisfied – or in other words, that in this case the RHS is also null. We will thus prove that if $\Lambda_\Gamma^{M^\beta}(\vec{q}) = \Lambda_\Gamma^{M^\beta}(\vec{r}) \; \forall M^\beta \notin \mathcal{P}^{\mathrm{str}}(N^\alpha)$ does not hold, then (C.64) is null, and thus the RHS in (C.63) is null as well.

We suppose (C.64) is not null, and take $M^\beta \notin \mathcal{P}^{\mathrm{str}}(N^\alpha)$ such that $\Lambda_\Gamma^{M^\beta}(\vec{q}) = 1$. Taking $A \in \mathrm{out}(M)$, and denoting $O := \mathtt{head}(A)$ and γ such that $\Lambda_\Gamma^{O^\gamma}(\vec{q}) = 1$, we have: either $O^\gamma \in \mathcal{P}^{\mathrm{str}}(N^\alpha)$, in which case $k_A = l_A$ by the penultimate term in (C.64); or $O^\gamma \notin \mathcal{P}^{\mathrm{str}}(N^\alpha)$, in which case $k_A = l_A$ by the last term in (C.64). Thus we have $k_A = l_A \forall A \in \mathrm{out}(M)$, and thus $\Lambda_\Gamma^{M^\beta}(\vec{r}) = 1$. Symmetrically, $\Lambda_\Gamma^{M^\beta}(\vec{r}) = 1$ implies $\Lambda_\Gamma^{M^\beta}(\vec{q}) = 1$, so we indeed get $\Lambda_\Gamma^{M^\beta}(\vec{r}) = \Lambda_\Gamma^{M^\beta}(\vec{q})$.

Therefore, (C.63) holds for $\vec{q}$ satisfying $\Lambda_\Gamma^{N^\alpha}(\vec{q}) = 1$. We can thus finally compute

$$
\mathcal{V}_0^\dagger[f_{\text{pad}}] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha)
$$

$$
= \sum_{\substack{\vec{q},\vec{r} \\ \Lambda_\Gamma^{N^\alpha}(\vec{q})=1}} \left(\bigotimes_{O^\gamma \in \text{Bran}_\Gamma} \pi_{O_{\text{out}}^\gamma}^{r^{O^\gamma}} \right) \circ \mathcal{V}_0^\dagger[f_{\text{pad}}] \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha) \circ \left(\bigotimes_{O^\gamma \in \text{Bran}_\Gamma} \pi_{O_{\text{out}}^\gamma}^{q^{O^\gamma}} \right)
$$

$$
\overset{(C.63)}{=} \sum_{\substack{\vec{q},\vec{r} \\ \Lambda_\Gamma^{N^\alpha}(\vec{q})=1}} F^{(r^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)},(q^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)}}
$$

$$
\otimes \left(\bigotimes_{M^\beta \notin \mathcal{P}^{\text{str}}(N^\alpha)} \pi_{M_{\text{out}}^\beta}^{q^{M^\beta}} \right) \cdot \prod_{O^\gamma \notin \mathcal{P}^{\text{str}}(N^\alpha)} \delta_{q^{O^\gamma},r^{O^\gamma}}
$$

$$
= \sum_{\substack{(q^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)} \\ (r^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)}}} \left(F^{(r^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)},(q^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)}} \otimes \sum_{\substack{(q^{O^\gamma})_{O^\gamma \notin \mathcal{P}^{\text{str}}(N^\alpha)} \\ \Lambda_\Gamma^{N^\alpha}(\vec{q})=1}} \left(\bigotimes_{M^\beta \notin \mathcal{P}^{\text{str}}(N^\alpha)} \pi_{M_{\text{out}}^\beta}^{q^{M^\beta}} \right) \right)
$$

$$
= \left(\sum_{\substack{(q^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)} \\ (r^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)}}} F^{(r^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)},(q^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)}} \right) \circ \left(\sum_{\substack{(s^{O^\gamma})_{O^\gamma \in \text{Bran}_\Gamma} \\ \Lambda_\Gamma^{N^\alpha}(\vec{s})=1}} \bigotimes_{M^\beta \notin \mathcal{P}^{\text{str}}(N^\alpha)} \pi_{M_{\text{out}}^\beta}^{s^{M^\beta}} \right)_{\text{pad}}
$$

$$
= \left(\sum_{\substack{(q^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)} \\ (r^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)}}} F^{(r^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)},(q^{O^\gamma})_{O^\gamma \in \mathcal{P}^{\text{str}}(N^\alpha)}} \right) \circ \zeta_{\text{pad}}^{\text{out}}(N^\alpha) \, ;
$$

$$ \tag{C.65} $$

denoting the left-hand factor as f' yields (C.37).

H7 The proof of (H7) is the symmetric of that of (H6).

Proof of the induction step

We suppose the induction hypotheses are all satisfied up to step i. We write $M^\beta :=$ $B(i+1)$, the branch we have to refill in this induction step.

   We first consider the case: neither i nor $i+1$ are special steps. Note that, because the branches have been ordered so that all branches of a same layer are next to each other, the fact that $i+1$ is not a special step entails: M^β is in a red layer $\implies \mathcal{P}_i(M^\beta) = \emptyset$.

H1 Let us first prove H1 at step $i+1$. From (C.32) and (H5) applied to $Q = \{M^\beta\}$, we have

$$\mathcal{S}_{\text{pad}}[(V_{N,i})_N] = \zeta_{i,\text{pad}}^{\text{in}}(M^\beta) \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (V_{M,i}^\beta)] \circ \zeta_{i,\text{pad}}^{\text{out}}(M^\beta)$$
$$+ \bar{\zeta}_{i,\text{pad}}^{\text{in}}(M^\beta) \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (\bar{V}_{M,i}^\beta)] \circ \bar{\zeta}_{i,\text{pad}}^{\text{out}}(M^\beta). \tag{C.66}$$

Furthermore,

$$\mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (V_{M,i+1}^\beta)] = \text{Tr}_{M_{\text{out}}^\beta}[U_{\text{pad}}^\beta \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (V_{M,i}^\beta)]], \tag{C.67a}$$

$$\mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (\bar{V}_{m,i+1}^\beta)] = \frac{1}{\dim(M^\beta)} \text{Tr}_{M_{\text{out}}^\beta}[\Theta_{M^\beta,\text{pad}}^\dagger \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (\bar{V}_{M,i}^\beta)]], \tag{C.67b}$$

so, because $\zeta_i^{\text{in}}(M^\beta)$ doesn't act on M_{in}^β, and $\zeta_i^{\text{out}}(M^\beta)$ doesn't act on M_{out}^β,

$$\mathcal{S}_{\text{pad}}[(V_{N,i+1})_N] = \mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (V_{M,i+1}^\beta)] + \mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (\bar{V}_{M,i+1}^\beta)]$$
$$= \zeta_{i,\text{pad}}^{\text{in}}(M^\beta) \circ \text{Tr}_{M_{\text{out}}^\beta}[U_{\text{pad}}^\beta \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (V_{M,i}^\beta)]] \circ \zeta_{i,\text{pad}}^{\text{out}}(M^\beta)$$
$$+ \bar{\zeta}_{i,\text{pad}}^{\text{in}}(M^\beta) \circ \frac{1}{\dim(M^\beta)} \text{Tr}_{M_{\text{out}}^\beta}[\Theta_{M^\beta,\text{pad}}^\dagger \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (\bar{V}_{M,i}^\beta)]] \circ \bar{\zeta}_{i,\text{pad}}^{\text{out}}(M^\beta). \tag{C.68}$$

Therefore, $\mathcal{S}_{\text{pad}}[(V_{N,i+1})_N]$ can be decomposed into two terms: one that can be considered as a linear map from the subspace of $\mathcal{H}_i^{\text{out}}$ defined by the projector $\zeta_{i,\text{pad}}^{\text{out}}(M^\beta)$, to the subspace of $\mathcal{H}_i^{\text{in}}$ defined by the projector $\zeta_{i,\text{pad}}^{\text{in}}(M^\beta)$; and one that can be considered a linear map from, and to, the subspaces orthogonal to these. We now have to prove that each of these two terms is unitary.

We start with the first term. (H6) implies that $U_{\text{pad}}^\beta \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (V_{M,i}^\beta)]$ features no causal influence from M_{out}^β to M_{in}^β, via the characterisation of causal influence in terms of algebras [5] (note that it makes sense to talk about the factors M_{out}^β and M_{in}^β of its input and output spaces because the $\zeta(M^\beta)$'s do not act on these). Therefore, one can find a unitary causal decomposition of it as $W^2 \circ (\text{SWAP}_{M_{\text{out}}^\beta, M_{\text{in}}^\beta} \otimes \mathbb{1}) \circ W^1$, where W^1 doesn't act on M_{out}^β and W^2 doesn't act on M_{in}^β. The first term in (C.68) – with its input and output spaces suitably restricted – is thus of the form $W^2 \circ (U^\beta \otimes \mathbb{1}) \circ W^1$, which is unitary.

As for the second term, one can see from the definition of the $V_{M,i}^\alpha$'s that $\mathcal{S}_{\text{pad}}[(V_{N,i})_{N \neq M} \times (\bar{V}_{M,i}^\beta)]$ is of the form $\Theta_{M^\beta} \otimes W$, with W a unitary (once restricted to the suitable subspaces). Therefore, the term can simply be rewritten as W.

We have therefore proven (H1) at rank $i+1$.

A Lemma. Before turning to the other induction hypotheses, we prove a Lemma that we will need to use a few times to compute how $\mathcal{V}_{i+1}^\dagger$ acts on sufficiently well-behaved linear operators.

Lemma C.2.5. *Let $g \in \mathrm{Lin}[\mathcal{H}_i^{\mathrm{in}}]$, not acting (i.e. acting trivially) on M_{in}^{β}, commuting with $\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\beta})$, and satisfying: $\mathcal{V}_i^{\dagger}[g] \circ \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{out}}(M^{\beta})$ doesn't act on M_{out}^{β}. We fix an orthonormal (with respect to the Hilbert-Schmidt inner product) basis $(E_m)_{1 \leq m \leq \dim(M_{\mathrm{out}}^{\beta})^2}$ of $\mathrm{Lin}[\mathcal{H}_{M_{\mathrm{out}}^{\beta}}]$, with $E_0 = \mathbb{1}$, and decompose $\mathcal{V}_i^{\dagger}[g]$ as*

$$\mathcal{V}_i^{\dagger}[g] = \sum_m \chi_m \otimes E_m \,, \tag{C.69}$$

with the χ_m's acting on $\mathcal{H}_P \otimes \left(\bigotimes_{O^{\gamma} > B(i+1)} \mathcal{H}_{O_{\mathrm{out}}^{\gamma}} \right)$. With padding, we can also write $\mathcal{V}_i^{\dagger}[g] = \sum_m \chi_{m,\mathrm{pad}} \circ E_{m,\mathrm{pad}}$, with the terms commuting. We then have

$$\mathcal{V}_{i+1}^{\dagger}[g] = \chi_{0,\mathrm{pad}} + \sum_{m \neq 0} E'_{m,\mathrm{pad}} \circ \chi_{m,\mathrm{pad}} \,, \tag{C.70}$$

where the E'_m's are defined, through the use of (H6) at step i, by $\mathcal{V}_i^{\dagger}[(U^{\beta\dagger} E_m U^{\beta})_{\mathrm{pad}}] \circ \zeta_{i,\mathrm{pad}}^{\mathrm{out}}(M^{\beta}) = E'_{m,\mathrm{pad}} \circ \zeta_{i,\mathrm{pad}}^{\mathrm{out}}(M^{\beta})$, with the E'_m's only acting on $\mathcal{H}_P$ (because $\mathcal{P}_i^{\mathrm{str}}(M^{\beta}) = \varnothing$).

Proof. We will compute $\mathcal{V}_{i+1}^{\dagger}[g]$ by looking at how g 'moves through' $\mathcal{S}_{\mathrm{pad}}[(V_{N,i+1})_N]$. First, we rewrite (C.68) more compactly as

$$
\begin{aligned}
&\mathcal{S}_{\mathrm{pad}}[(V_{N,i+1})_N] \\
&= \mathrm{Tr}_{M_{\mathrm{out}}^{\beta}} \left[\left(\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\beta}) \otimes U_{\mathrm{pad}}^{\beta} + \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\beta}) \otimes \frac{1}{\dim(M^{\beta})} \Theta_{M^{\beta},\mathrm{pad}}^{\dagger} \right) \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i})_N] \right] \,.
\end{aligned}
\tag{C.71}
$$

Thus (because g doesn't act on M_{in}^{β}, and commutes with $\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\beta})$),

$$
\begin{aligned}
&g \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i+1})_N] \\
&= g \circ \mathrm{Tr}_{M_{\mathrm{out}}^{\beta}} \left[\left(\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\beta}) \circ U_{\mathrm{pad}}^{\beta} + \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\beta}) \circ \frac{1}{\dim(M^{\beta})} \Theta_{M^{\beta},\mathrm{pad}}^{\dagger} \right) \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i})_N] \right] \\
&= \mathrm{Tr}_{M_{\mathrm{out}}^{\beta}} \left[\left(\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\beta}) \circ U_{\mathrm{pad}}^{\beta} + \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\beta}) \circ \frac{1}{\dim(M^{\beta})} \Theta_{M^{\beta},\mathrm{pad}}^{\dagger} \right) \circ g \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i})_N] \right] \\
&= \mathrm{Tr}_{M_{\mathrm{out}}^{\beta}} \left[\left(\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\beta}) \circ U_{\mathrm{pad}}^{\beta} + \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\beta}) \circ \frac{1}{\dim(M^{\beta})} \Theta_{M^{\beta},\mathrm{pad}}^{\dagger} \right) \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i})_N] \circ \mathcal{V}_i^{\dagger}[g] \right] \,.
\end{aligned}
\tag{C.72}
$$

We now consider the decomposition (C.69) of $\mathcal{V}_i^{\dagger}[g]$, and we look at

$$
\begin{aligned}
\sum_{m \neq 0} (\chi_{m,\mathrm{pad}} \circ \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{out}}(M^{\beta})) \otimes E_m &= \sum_{m \neq 0} (\chi_m \otimes E_m)_{\mathrm{pad}} \circ \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{out}}(M^{\beta}) \\
&= \mathcal{V}_i^{\dagger}[g] \circ \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{out}}(M^{\beta}) - (\chi_0 \otimes \mathbb{1}_{M_{\mathrm{out}}^{\beta}})_{\mathrm{pad}} \circ \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{out}}(M^{\beta}) \,.
\end{aligned}
\tag{C.73}
$$

Both terms of the second line's RHS act trivially on M_{out}^{β}: the first term by assumption, and the second because it is a composition of operators acting trivially on M_{out}^{β}. From the form of the LHS, we can thus deduce: $\forall m \neq 0, \chi_{m,\text{pad}} \circ \bar{\zeta}_{i,\text{pad}}^{\text{out}}(M^{\beta}) = 0$, which can be rewritten as

$$\forall m \neq 0, \chi_{m,\text{pad}} = \chi_{m,\text{pad}} \circ \zeta_{i,\text{pad}}^{\text{out}}(M^{\beta}). \tag{C.74}$$

In the same way we can prove that $\chi_{m,\text{pad}} = \zeta_{i,\text{pad}}^{\text{out}}(M^{\beta}) \circ \chi_{m,\text{pad}}$. We are now in a position to continue the computation started in (C.72); we write $\kappa_i^{\text{in}}(M^{\beta}) := \zeta_{i,\text{pad}}^{\text{in}}(M^{\beta}) \otimes U_{\text{pad}}^{\beta} + \bar{\zeta}_{i,\text{pad}}^{\text{in}}(M^{\beta}) \otimes \frac{1}{\dim(M^{\beta})}\Theta_{M^{\beta},\text{pad}}^{\dagger}$.

$$g \circ \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N]$$

$$\stackrel{\text{(C.74)}}{=} \text{Tr}_{M_{\text{out}}^{\beta}} \left[\left(\zeta_{i,\text{pad}}^{\text{in}}(M^{\beta}) \circ U_{\text{pad}}^{\beta} + \bar{\zeta}_{i,\text{pad}}^{\text{in}}(M^{\beta}) \circ \frac{1}{\dim(M^{\beta})}\Theta_{M^{\beta},\text{pad}}^{\dagger} \right) \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \circ \chi_{0,\text{pad}} \right]$$

$$+ \sum_{m \neq 0} \text{Tr}_{M_{\text{out}}^{\beta}} \left[\zeta_{i,\text{pad}}^{\text{in}}(M^{\beta}) \circ U_{\text{pad}}^{\beta} \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \circ \chi_{m,\text{pad}} \circ E_{m,\text{pad}} \right]$$

$$= \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N] \circ \chi_{0,\text{pad}}$$

$$+ \sum_{m \neq 0} \text{Tr}_{M_{\text{out}}^{\beta}} \left[E_{m,\text{pad}} \circ \zeta_{i,\text{pad}}^{\text{in}}(M^{\beta}) \circ U_{\text{pad}}^{\beta} \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \circ \chi_{m,\text{pad}} \right]$$

$$= [\ldots] + \sum_{m \neq 0} \text{Tr}_{M_{\text{out}}^{\beta}} \left[\zeta_{i,\text{pad}}^{\text{in}}(M^{\beta}) \circ U_{\text{pad}}^{\beta} \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \circ \mathcal{V}_i^{\dagger}[(U^{\beta^{\dagger}} E_m U^{\beta})_{\text{pad}}] \right] \circ \chi_{m,\text{pad}}$$

$$= [\ldots] + \sum_{m \neq 0} \text{Tr}_{M_{\text{out}}^{\beta}} \left[\kappa_{i,\text{pad}}^{\text{in}}(M^{\beta}) \circ \zeta_{i,\text{pad}}^{\text{in}}(M^{\beta}) \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \circ \mathcal{V}_i^{\dagger}[(U^{\beta^{\dagger}} E_m U^{\beta})_{\text{pad}}] \right] \circ \chi_{m,\text{pad}}$$

$$= [\ldots] + \sum_{m \neq 0} \text{Tr}_{M_{\text{out}}^{\beta}} \left[\kappa_{i,\text{pad}}^{\text{in}}(M^{\beta}) \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \circ \mathcal{V}_i^{\dagger}[(U^{\beta^{\dagger}} E_m U^{\beta})_{\text{pad}}] \circ \zeta_{i,\text{pad}}^{\text{out}}(M^{\beta}) \right] \circ \chi_{m,\text{pad}}$$

$$\stackrel{\text{(H6)}}{=} [\ldots] + \sum_{m \neq 0} \text{Tr}_{M_{\text{out}}^{\beta}} \left[\kappa_{i,\text{pad}}^{\text{in}}(M^{\beta}) \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \circ E'_{m,\text{pad}} \circ \zeta_{i,\text{pad}}^{\text{out}}(M^{\beta}) \right] \circ \chi_{m,\text{pad}}$$

$$= [\ldots] + \sum_{m \neq 0} \text{Tr}_{M_{\text{out}}^{\beta}} \left[\kappa_{i,\text{pad}}^{\text{in}}(M^{\beta}) \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \right] \circ E'_{m,\text{pad}} \circ \zeta_{i,\text{pad}}^{\text{out}}(M^{\beta}) \circ \chi_{m,\text{pad}}$$

$$\stackrel{\text{(C.71)}}{=} [\ldots] + \sum_{m \neq 0} \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N] \circ E'_{m,\text{pad}} \circ \zeta_{i,\text{pad}}^{\text{out}}(M^{\beta}) \circ \chi_{m,\text{pad}}$$

$$\stackrel{\text{(C.74)}}{=} [\ldots] + \sum_{m \neq 0} \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N] \circ E'_{m,\text{pad}} \circ \chi_{m,\text{pad}}$$

$$= \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N] \circ \left(\chi_{0,\text{pad}} + \sum_{m \neq 0} E'_{m,\text{pad}} \circ \chi_{m,\text{pad}} \right).$$

$$\tag{C.75}$$

In the previous computation, we used (H6) to replace $\mathcal{V}_i^{\dagger}[(U^{\beta^{\dagger}} E_m U^{\beta})_{\text{pad}}] \circ \zeta_{i,\text{pad}}^{\text{out}}(M^{\beta})$ with $E'_{m,\text{pad}} \circ \zeta_{i,\text{pad}}^{\text{out}}(M^{\beta})$, with the E'_m's only acting on $\mathcal{H}_P$ (because $\mathcal{P}_i^{\text{str}}(M^{\beta}) = \varnothing$). This then allowed us to get the term out of the trace. The computation allows us to conclude that (C.70) holds.

$\square$

H2 We now turn to (H2). We will take: $\forall N^\alpha > B(i+1), \zeta_{i+1}^{\mathrm{in}}(N^\alpha) := \zeta_i^{\mathrm{in}}(N^\alpha)$. There are two things to check in order to ensure that this makes sense. The first is that the $\zeta_i^{\mathrm{in}}(N^\alpha)$ are indeed all defined, which holds here because i is not a special step. The second thing to check is that for an arbitrary N^α, $\zeta_i^{\mathrm{in}}(N^\alpha)$ wasn't acting on M_{in}^β. This follows from the fact that $i+1$ is not a special step. Indeed, the way we defined the ordering of the branches ensures that $M^\beta \notin \mathcal{F}_i^{\mathrm{str}}(N^\alpha)$. This ensures that $\zeta_i^{\mathrm{in}}(N^\alpha)$ doesn't act on M_{in}^β if N^α is in a green layer; while if N^α is in a red layer, then the fact that $i+1$ is not a special step implies that M^β is not in this red layer, i.e. that $M^\beta \notin \mathcal{F}_i(N^\alpha)$ and thus that $\zeta_i^{\mathrm{in}}(N^\alpha)$ doesn't act on M_{in}^β.

We then want to define, from there, $\zeta_{i+1,\mathrm{pad}}^{\mathrm{out}}(N^\alpha) := \mathcal{V}_{i+1}^\dagger[\zeta_{i+1,\mathrm{pad}}^{\mathrm{in}}(N^\alpha)], \forall N^\alpha$. The fact (which derives from (H1)) that $\mathcal{V}_{i+1}$ is an isomorphism of operator algebras will then ensure that the $\zeta_{i+1,\mathrm{pad}}^{\mathrm{out}}$'s are pairwise commuting orthogonal projectors, as the $\zeta_{i+1,\mathrm{pad}}^{\mathrm{in}}$'s are. What is left to prove is that, fixing an N^α whose layer is green, $\mathcal{V}_{i+1}^\dagger[\zeta_{i+1,\mathrm{pad}}^{\mathrm{in}}(N^\alpha)]$ (which formally acts on the whole $\mathcal{H}_{i+1}^{\mathrm{out}}$) can indeed be seen as the padding of an operator acting on $\mathcal{H}_P \otimes \left(\bigotimes_{O^\gamma \in \mathcal{P}_{i+1}(N^\alpha)} \mathcal{H}_{O_{\mathrm{out}}^\gamma} \right)$ – i.e., that it acts trivially on other factors; and similarly, that for an N^α whose layer is red, $\mathcal{V}_{i+1}^\dagger[\zeta_{i+1,\mathrm{pad}}^{\mathrm{in}}(N^\alpha)]$ can be seen as only acting on $\mathcal{H}_P \otimes \left(\bigotimes_{O^\gamma \in \mathcal{P}_{i+1}^{\mathrm{str}}(N^\alpha)} \mathcal{H}_{O_{\mathrm{out}}^\gamma} \right)$.

For this, fixing an $N^\alpha > B(i+1)$, we will make use of Lemma C.2.5 to compute $\mathcal{V}_{i+1}^\dagger[\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(N^\alpha)]$. The latter satisfies the lemma's assumptions: $\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(N^\alpha)$ doesn't act on M_{in}^β and commutes with $\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^\beta)$ by (H1) at step i, and $\mathcal{V}_i^\dagger[\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(N^\alpha)] = \zeta_{i,\mathrm{pad}}^{\mathrm{out}}(N^\alpha)$, by (H3) at step i, satisfies: $\zeta_{i,\mathrm{pad}}^{\mathrm{out}}(N^\alpha) \circ \bar\zeta_{i,\mathrm{pad}}^{\mathrm{out}}(M^\beta)$ acts trivially on M_{out}^β.

By Lemma C.2.5, writing $\zeta_i^{\mathrm{out}}(N^\alpha) = \sum_m \chi_m \otimes E_m$, we can thus conclude

$$\mathcal{V}_{i+1}^\dagger[\zeta_{i+1,\mathrm{pad}}^{\mathrm{in}}(N^\alpha)] = \chi_{0,\mathrm{pad}} + \sum_{m \neq 0} E_{m,\mathrm{pad}}' \circ \chi_{m,\mathrm{pad}} . \tag{C.76}$$

If N^α is in a green layer, then in this expression, the χ_m's act on $\mathcal{H}_P \otimes \left(\bigotimes_{O^\gamma \in \mathcal{P}_{i+1}(N^\alpha)} \mathcal{H}_{O_{\mathrm{out}}^\gamma} \right)$ and the E_m''s act on $\mathcal{H}_P$; thus, $\mathcal{V}_{i+1}^\dagger[\zeta_{i+1,\mathrm{pad}}^{\mathrm{in}}(N^\alpha)]$ only acts non-trivially on $\mathcal{H}_P \otimes \left(\bigotimes_{O^\gamma \in \mathcal{P}_{i+1}(N^\alpha)} \mathcal{H}_{O_{\mathrm{out}}^\gamma} \right)$. If N^α is in a red layer, the same can be said replacing $\mathcal{P}$'s with $\mathcal{P}^{\mathrm{str}}$'s. This concludes the proof of (H2).

H3 The proof of (H3) is direct for the $\zeta_{i+1}^{\mathrm{in}}$'s, as they are equal to the ζ_i^{in}'s. For the $\zeta_{i+1}^{\mathrm{out}}$'s, fixing N^α and O^γ, one can compute $\zeta_{i+1,\mathrm{pad}}^{\mathrm{out}}(N^\alpha) \circ \bar\zeta_{i+1,\mathrm{pad}}^{\mathrm{out}}(O^\gamma) = \mathcal{V}_{i+1}^\dagger[\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(N^\alpha) \circ \bar\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(O^\gamma)]$ by once again invoking Lemma C.2.5, writing

$$\zeta_i^{\mathrm{out}}(N^\alpha) \circ \bar\zeta_i^{\mathrm{out}}(M^\beta) = \sum_m \xi_m \otimes E_m , \tag{C.77}$$

where the ξ_m's act trivially on O_{out}^γ because $\zeta_i^{\mathrm{out}}(N^\alpha) \circ \bar\zeta_i^{\mathrm{out}}(M^\beta)$ does, by (H3) at step i. $\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(N^\alpha) \circ \bar\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(O^\gamma)$ commutes with $\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^\beta)$ and doesn't act on M_{in}^β; to apply the Lemma, we thus have to prove that $\zeta_{i,\mathrm{pad}}^{\mathrm{out}}(N^\alpha) \circ \bar\zeta_{i,\mathrm{pad}}^{\mathrm{out}}(O^\gamma) \circ \bar\zeta_{i,\mathrm{pad}}^{\mathrm{out}}(M^\beta)$ acts trivially on M_{out}^β. This follows from the rewriting

$$\zeta_{i,\mathrm{pad}}^{\mathrm{out}}(N^\alpha) \circ \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{out}}(O^\gamma) \circ \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{out}}(M^\beta)$$
$$= \left(\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(N^\alpha) \circ \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{in}}(M^\beta)\right) \circ \left(\bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{out}}(M^\beta) - \zeta_{i,\mathrm{pad}}^{\mathrm{out}}(O^\gamma) \circ \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{out}}(M^\beta)\right), \tag{C.78}$$

all of the terms in which, one can conclude by (H3) at step i, act trivially on M_{out}^β. Lemma C.2.5 thus leads to

$$\zeta_{i+1,\mathrm{pad}}^{\mathrm{out}}(N^\alpha) \circ \bar{\zeta}_{i+1,\mathrm{pad}}^{\mathrm{out}}(O^\gamma) = \mathcal{V}_{i+1}^\dagger[\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(N^\alpha) \circ \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{in}}(O^\gamma)] = \xi_{0,\mathrm{pad}} + \sum_{m \neq 0} E'_{m,\mathrm{pad}} \circ \xi_{m,\mathrm{pad}}, \tag{C.79}$$

with neither the ξ_m's nor the E'_m's acting on O_{out}^γ, which concludes the proof of (H3).

H4 The proof of (H4) at step $i+1$ is immediate as it derives from (H4) at step i for the $\zeta_{i+1}^{\mathrm{in}}$'s, which are equal to the ζ_i^{in}'s.

H5 For the proof of (H5), we take $Q \subseteq \{B(i') \mid i' \geq i+1\}$ a set of branches on different nodes, and $\tilde{Q} \subseteq \mathtt{Nodes}_\Gamma$ and a function α such that $Q = \{N^{\alpha(N)} \mid N \in \tilde{Q}\}$. We will prove the version of (H5) written with $\zeta_{i+1}^{\mathrm{in}}$'s. We first consider the case $M \in \tilde{Q}$. Then by (H4) we have $\zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\alpha(M)}) = \zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^{\alpha(M)}) \circ \bar{\zeta}_{i,\mathrm{pad}}^{\mathrm{in}}(M^\beta)$, and we can therefore write

$$\prod_{N \in \tilde{Q}} \zeta_{i+1,\mathrm{pad}}^{\mathrm{in}}(N^{\alpha(N)}) \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i+1})_N]$$
$$= \prod_{N \in \tilde{Q}} \zeta_{i,\mathrm{pad}}^{\mathrm{in}}(N^{\alpha(N)}) \circ \zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^\beta) \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i+1})_N]$$
$$= \prod_{N \in \tilde{Q}} \zeta_{i,\mathrm{pad}}^{\mathrm{in}}(N^{\alpha(N)}) \circ \zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^\beta) \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i+1})_N]$$
$$= \prod_{N \in \tilde{Q}} \zeta_{i,\mathrm{pad}}^{\mathrm{in}}(N^{\alpha(N)}) \circ \zeta_{i,\mathrm{pad}}^{\mathrm{in}}(M^\beta) \circ \frac{1}{\dim(M^\beta))} \mathrm{Tr}_{M_{\mathrm{out}}^\beta}\left[\Theta_{M^\beta,\mathrm{pad}}^\dagger \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i})_N]\right]$$
$$= \prod_{N \in \tilde{Q}} \zeta_{i,\mathrm{pad}}^{\mathrm{in}}(N^{\alpha(N)}) \circ \frac{1}{\dim(M^\beta))} \mathrm{Tr}_{M_{\mathrm{out}}^\beta}\left[\Theta_{M^\beta,\mathrm{pad}}^\dagger \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i})_N]\right]$$
$$\overset{(\mathrm{H5})}{=} \frac{1}{\dim(M^\beta))} \mathrm{Tr}_{M_{\mathrm{out}}^\beta}\left[\Theta_{M^\beta,\mathrm{pad}}^\dagger \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i})_{N \notin \tilde{Q}} \times (V_{N,i}^{\alpha(N)})_{N \in \tilde{Q}}]\right]$$
$$= \frac{1}{\dim(M^\beta))} \mathrm{Tr}_{M_{\mathrm{out}}^\beta}\left[\Theta_{M^\beta,\mathrm{pad}}^\dagger \circ \Theta_{M^\beta,\mathrm{pad}} \circ \mathcal{S}_{\mathrm{pad}}[(V_{N,i+1})_{N \notin \tilde{Q}} \times (V_{N,i+1}^{\alpha(N)})_{N \in \tilde{Q}}]\right]$$
$$= \mathcal{S}_{\mathrm{pad}}[(V_{N,i+1})_{N \notin \tilde{Q}} \times (V_{N,i+1}^{\alpha(N)})_{N \in \tilde{Q}}]. \tag{C.80}$$

In the case $M \notin \tilde{Q}$, then defining $\alpha(M) := \beta$, we have

$$\prod_{N \in \tilde{Q}} \zeta_{i+1,\text{pad}}^{\text{in}}(N^{\alpha(N)}) \circ \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N]$$

$$= \text{Tr}_{M_{\text{out}}^{\beta}} \left[\prod_{N \in \tilde{Q} \cup \{M\}} \zeta_{i,\text{pad}}^{\text{in}}(N^{\alpha(N)}) \circ U_{\text{pad}}^{\beta} \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \right]$$

$$+ \frac{1}{\dim(M^{\beta})} \text{Tr}_{M_{\text{out}}^{\beta}} \left[\prod_{N \in \tilde{Q}} \zeta_{i,\text{pad}}^{\text{in}}(N^{\alpha(N)}) \circ \bar{\zeta}_{i,\text{pad}}^{\text{in}}(M^{\beta}) \circ \Theta_{M^{\beta},\text{pad}}^{\dagger} \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \right]$$

$$\overset{(\text{H5})}{=} \text{Tr}_{M_{\text{out}}^{\beta}} \left[U_{\text{pad}}^{\beta} \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_{N \notin \tilde{Q} \cup \{M\}} \times (V_{N,i}^{\alpha(N)})_{N \in \tilde{Q} \cup \{M\}}] \right]$$

$$+ \frac{1}{\dim(M^{\beta})} \text{Tr}_{M_{\text{out}}^{\beta}} \left[\Theta_{M^{\beta},\text{pad}}^{\dagger} \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_{N \notin \tilde{Q} \cup \{M\}} \times (V_{N,i}^{\alpha(N)})_{N \in \tilde{Q}} \times (\bar{V}_{M,i}^{\beta})] \right]$$

$$= \mathcal{S}_{\text{pad}}[(V_{N,i+1})_{N \notin \tilde{Q} \cup \{M\}} \times (V_{N,i+1}^{\alpha(N)})_{N \in \tilde{Q}} \times (V_{M,i}^{\beta})]$$

$$+ \mathcal{S}_{\text{pad}}[(V_{N,i+1})_{N \notin \tilde{Q} \cup \{M\}} \times (V_{N,i+1}^{\alpha(N)})_{N \in \tilde{Q}} \times (\bar{V}_{M,i}^{\beta})]$$

$$= \mathcal{S}_{\text{pad}}[(V_{N,i+1})_{N \notin \tilde{Q}} \times (V_{N,i+1}^{\alpha(N)})_{N \in \tilde{Q}}].$$

$$(\text{C.81})$$

H6   To prove (H6), we fix a branch $N^{\alpha} > B(i+1)$ in a green layer, and $f \in \text{Lin}[\mathcal{H}_{N_{\text{in}}^{\alpha}}]$. We first consider the case $N^{\alpha} \notin \mathcal{F}_i^{\text{str}}(M^{\beta})$. $\zeta_i^{\text{in}}(M^{\beta})$ then doesn't act on N_{in}^{α}: indeed, either M^{β} is in a green layer and $\zeta_i^{\text{in}}(M^{\beta})$ doesn't act outside of $\mathcal{F}_i^{\text{str}}(M^{\beta})$, or M^{β} is in a red layer and then, because $i+1$ is not a special step, N^{α} is not in this layer and thus $N^{\alpha} \notin \mathcal{F}_i(M^{\beta})$. Furthermore, as we saw that $\mathcal{S}_{\text{pad}}[(V_{N,i})_N)] \circ \bar{\zeta}_{i,\text{pad}}^{\text{out}}(M^{\beta})$ was of the form $W \otimes \Theta_{M^{\beta}}$, and f doesn't act on M_{in}^{β}, it follows that $\mathcal{V}_i^{\dagger}[f] \circ \bar{\zeta}_{i,\text{pad}}^{\text{out}}(M^{\beta})$ doesn't act on M_{out}^{β}. We can therefore apply Lemma C.2.5 and get

$$\mathcal{V}_{i+1}^{\dagger}[f_{\text{pad}}] = \phi_{0,\text{pad}} + \sum_{m \neq 0} E'_{m,\text{pad}} \circ \phi_{m,\text{pad}} \overset{(\text{H6})}{=} \sum_{m} \mathcal{V}_i^{\dagger}[(U^{\beta\dagger} E_m U^{\beta})_{\text{pad}}] \circ \phi_{m,\text{pad}}, \quad (\text{C.82})$$

where $\mathcal{V}_i^{\dagger}[f_{\text{pad}}] = \sum_m \phi_m \otimes E_m$. Furthermore, as we've seen, we have $\zeta_{i+1,\text{pad}}^{\text{out}}(N^{\alpha}) = \sum_n \mathcal{V}_i^{\dagger}[(U^{\beta\dagger} E_n U^{\beta})_{\text{pad}}] \circ \chi_n$. We are therefore led to

$$\mathcal{V}_{i+1}^{\dagger}[f_{\text{pad}}] \circ \zeta_{i+1,\text{pad}}^{\text{out}}(N^{\alpha}) = \sum_{mn} \phi_m \circ \chi_n \circ \mathcal{V}_i^{\dagger}[(U^{\beta\dagger} \circ E_m \circ E_n \circ U^{\beta})_{\text{pad}}]$$

$$= \left(\sum_{mn} \sigma_{lmn} \phi_m \circ \chi_n \right) \circ \sum_l \mathcal{V}_i^{\dagger}[(U^{\beta\dagger} \circ E_l \circ U^{\beta})_{\text{pad}}],$$

$$(\text{C.83})$$

where the σ_{lmn}'s are the structure constants on $\text{Lin}[M_{\text{out}}^{\beta}]$, i.e. $E_m \circ E_n = \sum_l \sigma_{lmn} E_l$. Yet (H6) at step i gives us that there exists f' acting on P and $\mathcal{P}_i^{\text{str}}(N^{\alpha})$ (and therefore not on M_{out}^{β}) such that $\mathcal{V}_i^{\dagger}[f_{\text{pad}}] \circ \zeta_{i,\text{pad}}^{\text{out}}(N^{\alpha}) = f'_{\text{pad}} \circ \zeta_{i,\text{pad}}^{\text{out}}(N^{\alpha})$, which can be rewritten as

$$\sum_l \left(\sum_{mn} \sigma_{lmn} \phi_m \circ \chi_n \right) \otimes E_l = \sum_l \left(f'_{\text{pad}} \circ \chi_l \right) \otimes E_l \,, \tag{C.84}$$

leading to

$$\forall l, \sum_{mn} \sigma_{lmn} \phi_m \circ \chi_n = f'_{\text{pad}} \circ \chi_l \,. \tag{C.85}$$

Reinserting this into (C.83), we find

$$\begin{aligned}
\mathcal{V}^\dagger_{i+1}[f_{\text{pad}}] \circ \zeta^{\text{out}}_{i+1,\text{pad}}(N^\alpha) &= f'_{\text{pad}} \circ \sum_l \chi_l \circ \mathcal{V}^\dagger_i[(U^{\beta^\dagger} \circ E_l \circ U^\beta)_{\text{pad}}] \\
&= f'_{\text{pad}} \circ \zeta^{\text{out}}_{i+1,\text{pad}}(N^\alpha) \,,
\end{aligned} \tag{C.86}$$

where f' acts on P and on $\mathcal{P}^{\text{str}}_i(N^\alpha)$, and the latter is equal to $\mathcal{P}^{\text{str}}_{i+1}(N^\alpha)$ as $M^\beta \notin \mathcal{P}^{\text{str}}_i(N^\alpha)$.

We now consider the case $N^\alpha \in \mathcal{F}^{\text{str}}_i(M^\beta)$. We will use the fact that (C.37) can be equivalently written as $\zeta^{\text{out}}_{i,\text{pad}}(N^\alpha) \circ \mathcal{V}^\dagger_i[f_{\text{pad}}] = f'_{\text{pad}} \circ \zeta^{\text{out}}_{i,\text{pad}}(N^\alpha)$; indeed, $\zeta^{\text{in}}_{i,\text{pad}}(N^\alpha)$ doesn't act on N^α_{in}, so f_{pad} and $\zeta^{\text{in}}_{i,\text{pad}}(N^\alpha)$ commute, so $\mathcal{V}^\dagger_i[f]$ and $\mathcal{V}^\dagger_i[\zeta^{\text{in}}_{i,\text{pad}}(N^\alpha)] = \zeta^{\text{out}}_{i,\text{pad}}(N^\alpha)$ commute as well. We write $\kappa^{\text{out}}_i(M^\beta) := \zeta^{\text{out}}_{i,\text{pad}}(M^\beta) \otimes U^\beta_{\text{pad}} + \bar{\zeta}^{\text{out}}_{i,\text{pad}}(M^\beta) \otimes \frac{1}{\dim(M^\beta)} \Theta^\dagger_{M^\beta,\text{pad}}$.

$$\begin{aligned}
&\zeta^{\text{out}}_{i+1,\text{pad}}(N^\alpha) \circ \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N]^\dagger \circ f_{\text{pad}} \\
&= \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N]^\dagger \circ \zeta^{\text{in}}_{i,\text{pad}}(N^\alpha) \circ f_{\text{pad}} \\
&= \text{Tr}_{M^\beta_{\text{in}}} \left[\kappa^{\text{out}}_{i,\text{pad}}(M^\beta)^\dagger \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N]^\dagger \right] \circ \zeta^{\text{in}}_{i,\text{pad}}(N^\alpha) \circ f_{\text{pad}} \\
&= \text{Tr}_{M^\beta_{\text{in}}} \left[\kappa^{\text{out}}_{i,\text{pad}}(M^\beta)^\dagger \circ \zeta^{\text{out}}_{i,\text{pad}}(N^\alpha) \circ \mathcal{V}^\dagger_i[f_{\text{pad}}] \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N]^\dagger \right] \\
&\stackrel{\text{(H6)}}{=} \text{Tr}_{M^\beta_{\text{in}}} \left[\kappa^{\text{out}}_{i,\text{pad}}(M^\beta)^\dagger \circ f'_{\text{pad}} \circ \zeta^{\text{out}}_{i,\text{pad}}(N^\alpha) \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N]^\dagger \right] \\
&= \text{Tr}_{M^\beta_{\text{in}}} \left[\kappa^{\text{out}}_{i,\text{pad}}(M^\beta)^\dagger \circ f'_{\text{pad}} \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N]^\dagger \right] \circ \zeta^{\text{in}}_{i+1,\text{pad}}(N^\alpha) \,,
\end{aligned} \tag{C.87}$$

from which we get

$$\begin{aligned}
&\zeta^{\text{out}}_{i+1,\text{pad}}(N^\alpha) \circ \mathcal{V}^\dagger_{i+1}[f_{\text{pad}}] \\
&= \zeta^{\text{out}}_{i+1,\text{pad}}(N^\alpha) \circ \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N]^\dagger \circ f_{\text{pad}} \circ \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N] \\
&= \text{Tr}_{M^\beta_{\text{in}}} \left[\kappa^{\text{out}}_{i,\text{pad}}(M^\beta)^\dagger \circ f'_{\text{pad}} \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N]^\dagger \right] \\
&\quad \circ \text{Tr}_{M^\beta_{\text{in}}} \left[\mathcal{S}_{\text{pad}}[(V_{N,i})_N] \circ \kappa^{\text{out}}_{i,\text{pad}}(M^\beta) \right] \circ \zeta^{\text{out}}_{i+1,\text{pad}}(N^\alpha) \,.
\end{aligned} \tag{C.88}$$

We will rewrite the traces in another way, defining $|\Phi^+(M^\beta)\rangle := \sum_k |k\rangle_{M^\beta_{\text{in}}} \otimes |k\rangle_{M^{\beta}{}'_{\text{in}}}$, where $M^{\beta}{}'_{\text{in}} \cong M^\beta_{\text{in}}$, and $(|k\rangle)_k$ is an arbitrary orthonormal basis. The above can then

be expressed as

$$\zeta_{i+1,\text{pad}}^{\text{out}}(N^\alpha) \circ \mathcal{V}_{i+1}^\dagger[f_{\text{pad}}]$$

$$= \langle\Phi^+(M^\beta)|_{\text{pad}} \circ \kappa_{i,\text{pad}}^{\text{out}}(M^\beta)^\dagger \circ f_{\text{pad}}' \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N]^\dagger \circ |\Phi^+(M^\beta)\rangle_{\text{pad}}$$

$$\circ \langle\Phi^+(M^\beta)|_{\text{pad}} \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N] \circ \kappa_{i,\text{pad}}^{\text{out}}(M^\beta) \circ |\Phi^+(M^\beta)\rangle_{\text{pad}} \circ \zeta_{i+1,\text{pad}}^{\text{out}}(N^\alpha) \quad \text{(C.89)}$$

$$= \langle\Phi^+(M^\beta)|_{\text{pad}} \circ \kappa_{i,\text{pad}}^{\text{out}}(M^\beta)^\dagger \circ f_{\text{pad}}' \circ \mathcal{V}_{i,\text{pad}}^\dagger \left[|\Phi^+(M^\beta)\rangle_{\text{pad}} \langle\Phi^+(M^\beta)|_{\text{pad}}\right]$$

$$\circ \kappa_{i,\text{pad}}^{\text{out}}(M^\beta) \circ |\Phi^+(M^\beta)\rangle_{\text{pad}} \circ \zeta_{i+1,\text{pad}}^{\text{out}}(N^\alpha).$$

In this expression, $\langle\Phi^+(M^\beta)|$ and $|\Phi^+(M^\beta)\rangle$ act on M_{out}^β and $M_{\text{out}}^{\beta\,'}$; $\kappa^{\text{out}}(M^\beta)$ acts on P, M_{out}^β / M_{in}^β (on its domain/codomain), and $\mathcal{P}_i(M^\beta) \subseteq \mathcal{P}_i^{\text{str}}(N^\alpha)$; f' acts on P and $\mathcal{P}_i^{\text{str}}(N^\alpha)$; and $\mathcal{V}_{i,\text{pad}}^\dagger \left[|\Phi^+(M^\beta)\rangle_{\text{pad}} \langle\Phi^+(M^\beta)|_{\text{pad}}\right]$ acts on P, M_{out}^β, $M_{\text{in}}^{\beta\,'}$ and $\mathcal{P}_i(M^\beta) \subseteq \mathcal{P}_i^{\text{str}}(N^\alpha)$. Their composition – which doesn't act on M_{out}^β and $M_{\text{out}}^{\beta\,'}$ as these are explicitly terminated by $\langle\Phi^+(M^\beta)|$ and $|\Phi^+(M^\beta)\rangle$ – thus acts trivially outside of P and $\mathcal{P}_i^{\text{str}}(N^\alpha) \setminus \{M^\beta\} = \mathcal{P}_{i+1}^{\text{str}}(N^\alpha)$. Therefore, we can write

$$\zeta_{i+1,\text{pad}}^{\text{out}}(N^\alpha) \circ \mathcal{V}_{i+1}^\dagger[f_{\text{pad}}] = f_{\text{pad}}'' \circ \zeta_{i+1,\text{pad}}^{\text{out}}(N^\alpha), \quad \text{(C.90)}$$

with $f'' \in \text{Lin}\left[\mathcal{H}_P \otimes \left(\bigotimes_{O^\gamma \in \mathcal{P}_{i+1}^{\text{str}}(N^\alpha)} \mathcal{H}_{O_{\text{out}}^\gamma}\right)\right]$.

H7 We take $N^\alpha > M^\beta$ in a red layer, and $f \in \text{Lin}[\mathcal{H}_{N_{\text{out}}^\alpha}]$. Because N^α is in a red layer and $i + 1$ is not a special step, we have $N^\alpha \notin \mathcal{P}_i(M^\beta)$. Thus f commutes with $\kappa_i^{\text{out}}(M^\beta)$, as the latter only acts non trivially on P, $\mathcal{P}_i(M^\beta)$ and M^β. Thus,

$$f_{\text{pad}} \circ \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N]^\dagger \circ \zeta_{i+1,\text{pad}}^{\text{in}}(N^\alpha)$$

$$= f_{\text{pad}} \circ \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N]^\dagger \circ \zeta_{i,\text{pad}}^{\text{in}}(N^\alpha)$$

$$= \text{Tr}_{M_{\text{in}}^\beta}\left[\kappa_{i,\text{pad}}^{\text{out}}(M^\beta)^\dagger \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N]^\dagger \circ \mathcal{V}_i^\dagger[f_{\text{pad}}] \circ \zeta_{i,\text{pad}}^{\text{in}}(N^\alpha)\right]$$

$$= \text{Tr}_{M_{\text{in}}^\beta}\left[\kappa_{i,\text{pad}}^{\text{out}}(M^\beta)^\dagger \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N]^\dagger \circ \zeta_{i,\text{pad}}^{\text{in}}(N^\alpha) \circ \mathcal{V}_i^\dagger[f_{\text{pad}}]\right] \quad \text{(C.91)}$$

$$\overset{\text{(H7)}}{=} \text{Tr}_{M_{\text{in}}^\beta}\left[\kappa_{i,\text{pad}}^{\text{out}}(M^\beta)^\dagger \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N]^\dagger \circ \zeta_{i,\text{pad}}^{\text{in}}(N^\alpha) \circ f_{\text{pad}}'\right]$$

$$= \text{Tr}_{M_{\text{in}}^\beta}\left[\kappa_{i,\text{pad}}^{\text{out}}(M^\beta)^\dagger \circ \mathcal{S}_{\text{pad}}[(V_{N,i})_N]^\dagger\right] \circ \zeta_{i,\text{pad}}^{\text{in}}(N^\alpha) \circ f_{\text{pad}}'$$

$$= \mathcal{S}_{\text{pad}}[(V_{N,i+1})_N]^\dagger \circ \zeta_{i,\text{pad}}^{\text{in}}(N^\alpha) \circ f_{\text{pad}}',$$

where f' acts on $\mathcal{F}_i^{\text{str}}(N^\alpha) = \mathcal{F}_{i+1}^{\text{str}}(N^\alpha)$. We can use this to find (noting that $\mathcal{V}_{i+1}[f]$ and $\zeta_{i+1,\text{pad}}^{\text{in}}(N^\alpha)$ commute because f and $\zeta_{i+1,\text{pad}}^{\text{out}}(N^\alpha)$ do)

$$\zeta_{i+1,\text{pad}}^{\text{in}}(N^\alpha) \circ \mathcal{V}_{i+1}[f_{\text{pad}}] = \mathcal{V}_{i+1}[f_{\text{pad}}] \circ \zeta_{i+1,\text{pad}}^{\text{in}}(N^\alpha) = \zeta_{i+1,\text{pad}}^{\text{in}}(N^\alpha) \circ f_{\text{pad}}'. \quad \text{(C.92)}$$

The special steps The previous proofs were relying on the assumption that neither i nor $i+1$ were special steps. We now consider the other cases. Note first that the proof of (H1) presented earlier is valid in these cases as well.

We start with the case: $i+1$ is a special step (regardless of the status of i). One then only has to define, and check the properties of, the $\zeta_{i+1}(N^\alpha)$'s for $N^\alpha \in \mathcal{L}_{i+1}(M^\beta)$. Note that for such N^α's, the $\zeta_i(N^\alpha)$'s were defined at step i; indeed, either i is not a special step and all the ζ_i's were defined, or i is a special step, which entails that $\mathcal{L}_{i+1}(M^\beta) \subset \mathcal{L}_i(B(i))$, and the ζ_i's were defined for elements of this latter set.

One can then follow a proof strategy that is a time-reversed version of the one presented earlier, except that only the N^α's in $\mathcal{L}_{i+1}(M^\beta)$ are considered. Namely, we will define, for $N^\alpha \in \mathcal{L}_{i+1}(M^\beta)$, $\zeta_{i+1}^{\text{out}}(N^\alpha) := \zeta_i^{\text{out}}(N^\alpha)$ and $\zeta_{i+1,\text{pad}}^{\text{in}}(N^\alpha) := \mathcal{V}_i[\zeta_{i+1,\text{pad}}^{\text{out}}(N^\alpha)]$, and the rest of the proof can be obtained by following the earlier proof, simply replacing in's with out's, looking at daggered versions of maps, etc. Indeed, the induction hypotheses are fully invariant under time-symmetry, except for one crucial thing: the fact that, when looking in the forward direction, all branches of the layers in the strict past of the branch under consideration have been refilled already, and thus have no ζ's. Here, however, we are only redefining, and proving properties of, the $\zeta_{i+1}(N^\alpha)$'s of the layer under consideration; everything thus goes as if the branches in its strict future didn't exist. Moreover, the fact that $i+1$ is a special step implies that $B(i+1)$ is in a red layer, which means that, when considering things from a time-reversed perspective, $B(i+1)$ is in a green layer and thus neither i not $i+1$ are special steps. Thus, for the purposes of defining these $\zeta_{i+1}(N^\alpha)$'s, the situation is exactly symmetric to the one considered previously.

A final case to consider is: i is a special step but $i+1$ is not. In this case, $B(i)$ and $M^\beta = B(i+1)$ are in the same red layer, but $B(i+2)$ and the rest of the $N^\alpha > B(i+1)$ aren't. The interpretation is that we just finished filling up the branches of a red layer, a procedure during which we didn't define ζ's for the branches above it; so that we now have to redefine them. The strategy for this case is to define the $\zeta_{i+1}^{\text{in}}(N^\alpha)$'s to be equal, not to the $\zeta_i^{\text{in}}(N^\alpha)$'s – which were not defined –, but to the $\zeta_j^{\text{in}}(N^\alpha)$, where j is the latest step that was not special, i.e. the latest step at which these were defined. $B(j)$ is then the first branch of the red layer we finished refilling.

One can then follow a strategy similar to the previous proof, now deriving that (H2)-(H7) hold at step $i+1$ from the fact that they hold at step j. Let us highlight the main steps. First, from (C.68) holding at all steps between j and $i+1$, we can deduce

$$\mathcal{S}_{\text{pad}}[(V_{N,i+1})_N] = \text{Tr}_{B(t)^{\text{in}},\, j<t\leq i+1}\left[\mathcal{S}_{\text{pad}}[(V_{N,j})_N] \circ \left(\prod_{t=j+1}^{i+1} \kappa_{j,\text{pad}}^{\text{out}}(B(t))\right)\right], \quad \text{(C.93)}$$

where we also used the fact that, due to how we defined the ζ^{out}'s to remain the same when filling up a red layer, we have $\forall t \in [\![j+1, i+1]\!], \kappa_t^{\text{out}}(B(t)) = \kappa_j^{\text{out}}(B(t))$.

For (H2), we fix $N^\alpha > B(i+1)$; note that we then have $N^\alpha \in \mathcal{F}_i^{\text{str}}(B(i+1))$, because $B(i+1)$ is the last branch in its (red) layer. As before, we have to prove that, defining $\zeta_{i+1,\text{pad}}^{\text{in}}(N^\alpha) := \zeta_{j,\text{pad}}^{\text{in}}$ and $\zeta_{i+1,\text{pad}}^{\text{out}}(N^\alpha) := \mathcal{V}^{i+1}[\zeta_{i+1,\text{pad}}^{\text{in}}(N^\alpha)]$, the latter doesn't act outside of P and $\mathcal{P}_{i+1}(N^\alpha)$ (or $\mathcal{P}_{i+1}^{\text{str}}(N^\alpha)$ if N^α is in a red layer). Using (C.93) and techniques similar to before, we are led to

$$
\mathcal{V}_{i+1}^\dagger[\zeta_{j,\text{pad}}^{\text{in}}(N^\alpha)] = \left(\prod_{t=j+1}^{i+1} \langle \phi^+(B(t))|_{\text{pad}} \right) \circ \left(\prod_{t=j+1}^{i+1} \kappa_{j,\text{pad}}^{\text{out}}(B(t))^\dagger \right)
$$
$$
\circ \mathcal{V}_{j,\text{pad}}^\dagger \left[\prod_{t=j+1}^{i+1} |\Phi^+(B(t))\rangle_{\text{pad}} \langle \Phi^+(B(t))|_{\text{pad}} \right] \circ \zeta_{j,\text{pad}}^{\text{out}}(N^\alpha) \quad \text{(C.94)}
$$
$$
\circ \left(\prod_{t=j+1}^{i+1} \kappa_{j,\text{pad}}^{\text{out}}(B(t)) \right) \circ \left(\prod_{t=j+1}^{i+1} |\phi^+(B(t))\rangle_{\text{pad}} \right),
$$

in which $\zeta_{j,\text{pad}}^{\text{out}}(N^\alpha)$ acts only on P and $\mathcal{P}_j(N^\alpha)$ ($\mathcal{P}_j^{\text{str}}(N^\alpha)$ if N^α is in a red layer), and the other terms act only on $\mathcal{L}(B(i+1))$ and on P. Given that all the wires in $\mathcal{L}(B(i+1))$ are explicitly terminated by the ϕ^+'s, it follows that $\mathcal{V}_{i+1}^\dagger[\zeta_{j,\text{pad}}^{\text{in}}(N^\alpha)]$ only acts on P and on $\mathcal{P}_j(N^\alpha) \setminus \mathcal{L}(B(i+1)) = \mathcal{P}_{i+1}(N^\alpha)$ (or $\mathcal{P}_j^{\text{str}}(N^\alpha) \setminus \mathcal{L}(B(i+1)) = \mathcal{P}_{i+1}^{\text{str}}(N^\alpha)$ if N^α is in a red layer).

The proof of (H3) is fully analogous: computing $\mathcal{V}_{i+1}^\dagger[\zeta_{j,\text{pad}}^{\text{in}}(N^\alpha) \circ \bar{\zeta}_{j,\text{pad}}^{\text{in}}(M^\beta)]$ leads to (C.94) with $\zeta_{j,\text{pad}}^{\text{out}}(N^\alpha)$ replaced with $\zeta_{j,\text{pad}}^{\text{out}}(N^\alpha) \circ \bar{\zeta}_{j,\text{pad}}^{\text{out}}(M^\beta)$, so that invoking (H3) at step j leads to (H3) at step $i+1$. (H4), as before, is direct, and the proof of (H5) is analogous to the one for the non-special cases.

For the proof of (H6), we take $N^\alpha > B(i+1)$ in a green layer and $f \in \text{Lin}[\mathcal{H}_{N_{\text{in}}^\alpha}]$. Then, the computation is similar to (C.87), (C.88) and (C.89), yielding

$$
\zeta_{i+1,\text{pad}}^{\text{out}}(N^\alpha) \circ \mathcal{V}_{i+1}^\dagger[f_{\text{pad}}]
$$
$$
= \left(\prod_{t=j+1}^{i+1} \langle \phi^+(B(t))|_{\text{pad}} \right) \circ \left(\prod_{t=j+1}^{i+1} \kappa_{j,\text{pad}}^{\text{out}}(B(t))^\dagger \right) \circ \mathcal{V}_{j,\text{pad}}^\dagger \left[\prod_{t=j+1}^{i+1} |\Phi^+(B(t))\rangle_{\text{pad}} \langle \Phi^+(B(t))|_{\text{pad}} \right]
$$
$$
\circ f_{\text{pad}}' \circ \left(\prod_{t=j+1}^{i+1} \kappa_{j,\text{pad}}^{\text{out}}(B(t)) \right) \circ \left(\prod_{t=j+1}^{i+1} |\phi^+(B(t))\rangle_{\text{pad}} \right) \circ \zeta_{i+1,\text{pad}}^{\text{out}}(N^\alpha),
$$
$$
\text{(C.95)}
$$

where $f' \in \text{Lin}[\mathcal{H}_P \otimes (\otimes_{O^\gamma \in \mathcal{P}_j^{\text{str}}(N^\alpha)})]$ was defined through $\zeta_{j,\text{pad}}^{\text{out}}(N^\alpha) \circ \mathcal{V}_j^\dagger[f_{\text{pad}}] = f_{\text{pad}}' \circ \zeta_{j,\text{pad}}^{\text{out}}(N^\alpha)$ by using (H6) at step j. Once again, by looking at where the operators are acting, we can conclude that this defines a f'' acting only on P and on $\mathcal{P}_j^{\text{str}}(N^\alpha) \setminus \mathcal{L}(B(i+1)) = \mathcal{P}_{i+1}^{\text{str}}(N^\alpha)$.

Finally, for (H7), one can follow computations (C.91) and (C.92), to get

$$
\zeta_{i+1,\text{pad}}^{\text{in}}(N^\alpha) \circ \mathcal{V}_{i+1}[f_{\text{pad}}] = \zeta_{j,\text{pad}}^{\text{in}}(N^\alpha) \circ f_{\text{pad}}', \quad \text{(C.96)}
$$

where f', obtained by the use of (H7) at step j, only acts on $\mathcal{F}_j^{\text{str}}(N^\alpha) = \mathcal{F}_{i+1}^{\text{str}}(N^\alpha)$. This concludes the proof of the induction step.

Conclusion As the base case and induction step are true, the induction hypotheses are true at every step up to n. In particular, (H1) at step n then reads:

$$\mathcal{S}[(U_N)_N] \text{ is unitary.} \tag{C.97}$$

As this was done for $\mathcal{S} = \mathcal{S}_{(\Gamma,(\lambda_N)_N)}$ for an arbitrary valid routed graph $(\Gamma, (\lambda_N)_N)$, and for an arbitrary collection of routed unitaries $U_N : \mathcal{H}_N^{\text{in}} \overset{\lambda_N}{\to} \mathcal{H}_N^{\text{out}}$ following the λ_N's, we can invoke Lemma C.2.2 and conclude that Theorem C.2.1 holds.

$\square$

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