学位論文

On the difference between positivity and complete positivity of maps in quantum theory

(量子写像における正値性と完全正値性の差異)

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Abstract

The composability of local systems in quantum theory places a non-trivial restriction on quantum state transformations. Transformations of quantum states have to be completely positive maps that transform quantum states to other valid quantum states even when the maps are applied on a part of entangled states. In contrast, positive maps are guaranteed to transform quantum states to other valid quantum states only when the input states are not entangled to other systems. On the other hand, positive and completely positive maps are also definable in classical probability theory where these two notions define the same class of maps. Therefore the gap between positive and completely positive maps characterises the fundamental difference between quantum and classical probability theories. In this thesis, we consider two kinds of theories that intermediates quantum and classical probability theories, and analyse the gap between positivity and completely positivity in these theories.

We first consider a variant of quantum theory where the input states of maps are provided with their finite clones. Positive maps that are not completely positive such as state transposition $\rho \mapsto \rho^{\mathrm{T}}$ cannot be realised in quantum mechanics since they do not transform entangled states to valid quantum states. It is still impossible to construct machines to realise the action of positive but not completely positive maps even on the restricted set of quantum states that are not correlated to other systems. We investigate the gap between positivity and completely positivity by analysing the realisability of the action of positive maps on the states uncorrelated to other systems with respect to the number of clones. The gap closes when an infinite number of clones is provided, in the sense that it is possible to extract the classical description of the original state from the clones, and to produce the output state of any positive map. In other words, the action of positive maps on the uncorrelated states become realisable much like classical probability theory, if an infinite number of clones is provided. We show that the gap does not completely close with the finite clones, by proving the necessity of infinitely many clones to realise a certain class of positive maps including state transposition.

A special attention is paid on a mapping $\mathcal{E} \mapsto \mathrm{T} \circ \mathcal{E} \circ \mathrm{T}$ on quantum channels $\mathcal{E}$ which we call channel transposition. Channel transposition can be regarded as a positive map on maps that are not completely positive, and we show that it is not physically realizable from finite replicas of the map. We find, however, a method to realise channel transposition on unitary transformations from finite replicas, and thus show some of the gap between positivity and complete positivity closes. We also provide a physical interpretation of this method in fermionic systems, and an application of this method for computation of entanglement.

We secondly consider topos quantum theory to generalize positive maps in classical probability theory. Topos quantum theory provides representations of quantum states as direct generalizations of the probability distribution, namely probability valuation. Category theory provides the canonical extension of this generalization to positive maps.

Before proceeding to the analysis on maps, we define composite systems in topos quantum theory and analyse the joint valuations therein since the defining

difference between positivity and complete positivity arises in composite systems. Our definition of composite systems leads to a bijective correspondence between joint valuations and positive over pure tensor states, rather than quantum states. Positive over pure tensor states have close relationship between positive quantum maps from which we deduce that positive quantum maps may all regarded as completely positive in topos quantum theory.

Instead of a direct analysis on the positive maps between valuations, we consider Markov chains in topos quantum theory, motivated from the fact that classical Markov chains are generated from positive maps. Again category theory provides a straightforward generalization of classical Markov chains to topos quantum theory. We show several properties shared by Markov chains of classical probability theory and topos quantum theory. We find, however, an incompatibility between these shared properties and the monogamy of quantum states that trivializes Markov chains in topos quantum theory to product states.

Denotations and abbreviations used in the thesis

$\mathbb{C}_d$	A standard d dimensional Hilbert space
$\mathcal{H},\ \mathcal{K}$	Hilbert spaces
$\mathcal{B}(\mathcal{H},\mathcal{K})$	The set of bounded linear operators from given Hilbert space $\mathcal{H}$ to $\mathcal{K}$
$\mathcal{B}(\mathcal{H})$	The set of bounded linear operators on given Hilbert space $\mathcal{H}$
A_{sa}	The self-adjoint part of given C*-algebra A
$\mathrm{Pos}(\mathcal{H})$	The set of positive semi-definite operators on given $\mathcal{H}$
$\mathcal{S}(\mathcal{H})$	The set of density operators on given $\mathcal{H}$
$\mathrm{CP}(\mathcal{B}(\mathcal{H}),\mathcal{B}(\mathcal{K}))$	The set of completely positive maps from $\mathcal{B}(\mathcal{H})$ to $\mathcal{B}(\mathcal{K})$
$\mathcal{D},\ \mathcal{E},\ \mathcal{F}$	Linear maps between considered operator spaces
Γ	A trace preserving completely positive map between considered operator spaces
$\mathcal{I}$	A quantum instrument between considered operator spaces
$-\otimes-$	Tensor product of Hilbert spaces, algebras, operators and linear maps, or a tensor product for the considered monoidal category
$\bullet$	Tensor product especially for copied Hilbert spaces and operators
$\lvert a\rvert$	Absolute value of given scalar a
$[O]_{ij}$	The i,j entry of given operator O with respect to considered basis
$O^\dagger$	The adjoint (involution) of given operator O
O^*	Complex conjugation of given operator or scalar O
$\lvert\psi^*\rangle$	Complex conjugation of vector $\lvert\psi\rangle$ in the considered basis
O^{T}	Transposition of given operator O
T	The transposition map on the considered operator space
$\mathrm{Tr}[O]$	Trace of given operator O
$\mathcal{H}^{\otimes n},\ O^{\otimes n},\ \Gamma^{\otimes n}$	The n-th tensor power of given Hilbert space $\mathcal{H}$, given operator O and given linear map Γ
$\mathbb{I}_{\mathcal{H}}$	The identity operator on given Hilbert space $\mathcal{H}$
$\mathrm{id}_{\mathcal{H}},\ \mathrm{id}_X$	The identity map from given $\mathcal{B}(\mathcal{H})$ to itself, and the identity morphism of given object X
$\mathcal{U}[O]$	Adjoint action of given operator $O:\mathcal{H}\to\mathcal{K}$ on operators on $\mathcal{H}$ (i.e. $\mathcal{U}[O](A)=OAO^\dagger$)
$\mathcal{D}\circ\mathcal{E},\ g\circ f$	Sequential composition of given linear maps $\mathcal{E}$ and $\mathcal{D}$ and given morphisms f and g
$\Phi_{\mathcal{H},\mathcal{H}'}$	The unnormalised density operator for the maximally entangled vector $\sum_i \lvert i,i\rangle$ between given two isomorphic Hilbert spaces $\mathcal{H}$ and $\mathcal{H}'$ in the considered basis
χ	The Choi isomorphism from linear maps to bipartite operators
$\widetilde{\mathcal{E}}$	The Choi operator for given linear map $\mathcal{E}$

Denotations and abbreviations used in the thesis

$\mathrm{SU}(d)$	The special unitary group of degree d
$X \to_{\mathcal{K}\ell} Y$	Kleisli morphism from object X to Y of a given monad with functor part T
$g \odot f$	Kleisli composition of Kleisli morphisms f and g
st, cst	The strength and costrength of the relevant strong monad, respectively
$\mathrm{dst}, \mathrm{dst}'$	Fubini maps of the relevant strong monad
i	The Fubini map of the relevant commutative monad (also used as an index)
Sets	The category of sets and functions
$\mathscr{D}$	The functor part of the distribution monad
$\mathrm{SWAP}_{\mathcal{H}\otimes\mathcal{H}'}$	The swap operator between given isomorphic Hilbert spaces $\mathcal{H}$ and $\mathcal{H}'$
$\mathcal{W}(\mathcal{H}_1 \otimes ... \otimes \mathcal{H}_m)$	The set of positive over pure tensor states on given tensor product Hilbert space $\mathcal{H}_1 \otimes ... \otimes \mathcal{H}_m$
σ_y	The Pauli Y operator with eigenvalues 1 and -1
Θ	The conjugation operator on the relevant Hilbert space with respect to the considered basis
$\Pi_{\mathcal{H}}$	The projection operator on given Hilbert subspace $\mathcal{H}$
S_m	The symmetry group of order m
$\mathrm{sgn}(\tau)$	The signature of given permutation τ
$\lvert\wedge_{i_1,...,i_m}\rangle$	The Slater determinant $\sum_{\tau\in\mathrm{S}_m} \mathrm{sgn}(\tau)\lvert\tau_{i_1}, ..., \tau_{i_m}\rangle$ of given orthonormal state vectors $\lvert i_j\rangle$ $(j = 1, ..., m)$
$\mathcal{H}^{\wedge n}$	The anti-symmetric subspace of given n-th tensor power $\mathcal{H}^{\otimes n}$
$a_{\lvert\psi\rangle}$	The annihilation operator that annihilates a fermion in given state $\lvert\psi\rangle \in \mathcal{H}$
$\lvert\mathrm{vac}\rangle$	A vacuum state of fermions
$\lvert\mathrm{occ}\rangle$	A completely occupied state $a^\dagger_{\lvert 1\rangle}...a^\dagger_{\lvert n\rangle}\lvert\mathrm{vac}\rangle$ of fermions
C, **D**	Categories
$\mathrm{Hom}_{\mathbf{C}}(X, Y)$	The set of morphisms from object X to Y in category **C**
cCstar	The category of unital commutative C*-algebras and *-homomorphisms
KCRegLoc	The category of compact, completely regular locales and continuous maps
KRegLoc	The category of compact regular locales and continuous maps
$\mathbf{C}_{\mathcal{T}}$	Category **C** internal to given topos $\mathcal{T}$
Σ_A	The Gelfand spectrum for given unital commutative C*-algebra A
Loc	The category of locales and continuous maps
$\mathscr{I}$	The functor assigning the locale of integrals for f-algebras
$\mathscr{V}$	The functor assigning the locale of valuations for locales

Denotations and abbreviations used in the thesis

$[\mathbf{C}, \mathbf{D}]$	The category with functors from given category $\mathbf{C}$ to $\mathbf{D}$ as objects and the natural transformations as morphisms
(T, η, μ)	A monad with functor T, unit η, and multiplication μ
$\prod_i X_i$	The cartesian product of given objects X_i in the relevant category
π_X	The projector of relevant cartesian product onto given object X
$\langle f, g \rangle$	The product of given morphisms f and g
CP	Completely Positive
TP	Trace Preserving
TNI	Trace Non-Increasing

Contents

Chapter 1

Introduction

Quantum physics asserts the existence of fundamentally distinct phenomena when compared to classical physics. In addition to the standard examples such as superposition, uncertainty relations and entanglement, quantum physics also alludes to the possibility of information protocols, such as quantum metrology [1, 2], quantum computation [3] and quantum cryptography [4], which would be otherwise nonexistent if limited to classical physics.

These differences between quantum and classical physics may be formulated by abstracting to information theoretic frameworks. In this case, classical physics is associated to classical probability theory, in which classical information theory is formulated. The abstraction of quantum physics has also been introduced in the literature, which in this thesis would be collectively referred to as "quantum theory" (see [3] or Sec. 1.1.2 for details). Quantum theory is capable of describing classical probability theory as a special case, while the opposite implication fails (see e.g. [5] for a more detailed explanation).

Notions of local systems and their composites appear both in information theoretic and physical arguments. Local system is a fundamental concept in information theory, when accessibility to certain parts of a large system is restricted. The notion of composite systems is used to describe the case where several parties have operational resources to manipulate their local systems and communicate among themselves. This calls for an appropriate method to compose several local systems to form a single system, namely, multipartite system. These notions of local and composite systems are also employed when discussing interactions and correlations on multipartite systems in general.

The notions of locality and composition are mathematically formulated in terms of product states and product state transformations to describe behaviours of composite systems whose marginals are mutually independent. In classical probability theory, systems are described by random variables, and their composite by direct products. In quantum theory, systems are described by Hilbert spaces, and their composite by tensor products.

The composability of local systems places a non-trivial restriction on quantum state transformations. Transformations of states of a physical system is represented by mathematical maps. States in quantum theory are density operators (i.e. positive and normalised matrices), and those in classical probaiblity theory are probability distributions. Those maps that transform any states on a single systems to another are said to be *positive* both in classical probability theory and quantum theory. Positivity seems to be a necessary requirement for a map to represent a physical transformation, that *per se* however, does not guarantee the soundness of a quantum theory as a physical theory when combined with notions of locality and composites. When a positive quantum map is applied on a part of entangled states, the density operator of the initial state results in an operator called *positive over pure tensor states*, which may not be a density operator, in general. Thus in quantum theory, we need an additional soundness condition called *completely positivity* that demands the maps to transform all the states of composite systems to another valid state, even when applied on parts of the composite systems. While any positive maps are also completely positive (CP) for classical probability theory, some positive maps are not CP in quantum theory. The soundness of maps in a single system implies global soundness for classical probability theory, but not quantum theory.

There are other ways to observe the theoretical gap between positive and CP quantum maps without involving entangled states. The Stinespring dilation implies that any positive map reduces to a unitary transformation on extended Hilbert spaces if and only if it is CP [6]. This implies that the action of a positive non-CP maps is not realisable by a *quantum manipulator*, a general devise obeying quantum theory, even for uncorrelated input quantum states on which all positive maps are sound. It is already known for more than a decade that a particular positive non-CP map, namely transposition, can be used to enhance the power of state discrimination even if it is applied on states with no entanglement [7]. This does not hold for CP maps.

Several positive non-CP maps still appear in physics, despite being unrealisable in the standard quantum theory. The action of antiunitary transformations on quantum states, perhaps not seemingly a positive map, is equivalent to transposition followed by unitary transformations. According to Wigner, any symmetry transformations on quantum states are either unitary or antiunitary [8]. Antiunitary symmetry transformations such as time-reversal and charge-conjugation are considered to be a fundamental symmetry in quantum field theory [9] while there is no quantum manipulator realising the transformations on given unknown quantum states. Antiunitary transformations also appear frequently in definitions of multipartite correlation measures (see Sec. 2.3.3 for details). Although the above examples are all related only to transposition, the property of general positive non-CP maps to transform entangled states to positive over pure tensor states is useful for deciding whether a given bipartite state is entangled [10, 11]. In addition, positive maps also correspond to some form of non-Markovian quantum processes describing state transformations of subsystems with initial correlations to other subsystems [12].

Our understanding on positive non-CP maps is still incomplete. For example, all the known "bound" entangled states [13] remain valid quantum states under transposition applied on a part, while there are on-going efforts to clarify the connection between the physical soundness of a quantum state under this "partial transposition" and the "boundedness" of its entanglement [14, 15]. Partly motivated from the same problem, the tensor stability property of positive non-CP maps has recently begun being analysed [16, 17]. A variant of degradable channels

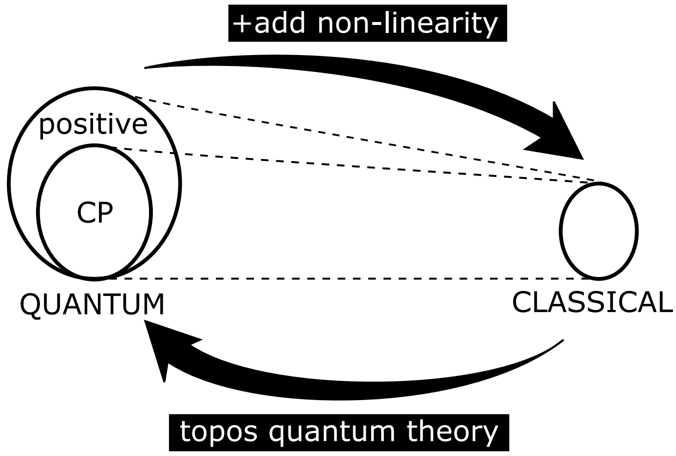

Figure 1.1: A schematic diagram of our two approaches to connect quantum and classical probability theories.

[18] called conjugate degradable channels is defined in Ref. [19] by using transposition, and relation to black hole theory is suggested in the literature [20]. It remains open, however, if there exist conjugate degradable channels that are not degradable [21]. Positive over pure tensor states may have multipartite correlations that cannot be simulated by quantum states, but there is no known information theoretic constraint to exclude these correlations [22].

All the preceding works raised in the previous two paragraphs do not have classical analogues. Positive non-CP maps are usually investigated inside quantum theory, since they do not exist in classical probability theory. At this point, it is difficult to assess the theoretical significance on the existence, or rather non-existence of positive non-CP maps in quantum theory, partly due to the fact that we only have two physically successful theories to compare. Perhaps there may be a physically sound theory that resembles classical probability theory without positive non-CP maps, or, conversely, a theory like a quantum theory but with positive non-CP maps. Should we succeed in formulating a sequence of physical theories that connects quantum theory and classical probability theory, the gap between positive and CP maps will emerge when the theory becomes closer to quantum theory, and disappear otherwise. Investigation of the gap between positive and CP maps in the *intermediate* theories would broaden our understanding of differences between quantum theory and classical probability theory. It would also provide us new insights into quantum theory itself regarding on positive non-CP maps.

In this thesis, we consider two approaches to connect quantum theory and classical probability theory, schematically represented in Fig. 1.1. On the first approach, we add non-linearity on quantum theory to make it closer to classical probability theory. In this case, we are interested in how the gap between positive and CP maps disappears, as we introduce non-linearity to quantum theory. On the second approach, we use topos quantum theory for generalising classical probability distributions to describe quantum states. In this case, we are interested in which of the positive and CP maps eventually appear in topos quantum theory when generalising classical probability theory. We shall introduce these two approaches separately in the following.

Adding non-linearity to quantum theory Linearity stemming from the use of Hilbert spaces is a characteristic principle of quantum theory that does not exist in classical probability theory. Quantum states exhibit superposition due to the linearity. On the other hand, linearity makes it impossible to realise non-linear maps such as state cloning of unknown pure states in quantum theory [23, 24], and only allows imperfect approximation of cloning [25]. Yet, perfect cloning of a probability distribution corresponding to a pure state is realisable in classical probability theory since there is no linearity constraint.

The first approach adds non-linearity to quantum theory in an attempt to bring it closer to classical probability theory. One way to add non-linear power to quantum theory is to allow *state cloning*, i.e. the power to make perfect copies of unknown quantum states. Indeed given an infinite number of clones of input state uncorrelated to other systems, any map on the state, even non-linear and/or positive non-CP, becomes realisable, by first measuring a suitable set of observables to identify the classical description of the input state (i.e. performing state tomography in the terminology of quantum information theory), and then creating the desired output state.[1] In this sense, quantum theory becomes equivalent to classical probability theory if an infinite number of clones are available, and separates as the number of clones decreases. The number of available clones in the theory serves as a parameter to characterise its closeness with respect to quantum and classical probability theory.

Motivated by this observation, we analyse the number of cloned input states uncorrelated to other systems which is required to realise positive non-CP maps. One can already find a discussion that introducing non-linearity might be helpful for inducing non-Markovian processes [26]. There is, however, a preceding work which suggests that transposition of a state is not deterministically realisable from any finite number of clones of unknown states [27] (see also [28]). In contrast to their work, we focus on probabilistic realisability from finite clones. Although the deterministic implementation of transposition is impossible, there remains the possibility to realise it probabilistically, i.e. with a probability smaller than 1 but not zero. We also consider probabilistic realisability of different positive non-CP maps other than transposition. Transposition seems the most difficult to realise among any positive non-CP maps since it transforms pure states to pure states. Other positive non-CP maps do not share this property, and thus we have the choice of adding noise to the cloned input states.

After analysing realisability of positive non-CP maps between states, we proceed to positive non-CP *supermaps*. Supermaps here refer to a class of maps that send state transformations into another state transformation. The notions of positivity and complete positivity may also be defined for supermaps. Similar to the case of maps, CP supermaps are physically realisable, while positive non-CP supermaps are not necessarily so (see Sec. 1.2.2 for more detail).

Just as the linearity constraint exists on quantum supermaps, a weak linearity constraint also exists in the classical counterpart. In analogy to the state cloning for maps, we can add non-linearity for supermaps by allowing *map replication*. If

[1]Note that the realisability of a positive map thus defined does not imply the realisability of the action of the positive map on marginal quantum systems. Such an action cannot be realisable since it may output an operator different from quantum states.

we have non-zero but finite replicas of an invertible transformations of probability distributions, it is possible to know the description of the transformation, and hence any non-linear supermaps are realisable. On the other hand, we require infinite replicas of invertible transformations to obtain its description in quantum theory. Thus we still require infinite replicas of unitary transformations to mimic the situation of classical probability theory where finite replicas of invertible maps are sufficient to realise any supermaps.

Following this observation, we analyse the number of replicas of maps required for realising positive non-CP quantum supermaps. The input maps of the supermaps are assumed to be uncorrelated to other systems so that the positive non-CP supermaps outputs valid quantum maps. We focus on a particular supermap which we call *channel transposition*. A trace preserving and CP (TPCP) map Γ sandwiched by transposition $\mathrm{T} \circ \Gamma \circ \mathrm{T}$ is a TPCP map. The supermap $\Gamma \mapsto \mathrm{T} \circ \Gamma \circ \mathrm{T}$ is a positive non-CP supermap that we call channel transposition. Somewhat surprisingly, channel transposition on 2-dimensional unitary transformations is known to be deterministically realisable without replicated unitary transformation, while we need infinite clones for 2-dimensional state transposition. A recent work suggests that deterministic channel transposition on unitary transformation is impossible without replicas if the dimension of unitary transformation is larger than 3 [29]. We investigate the probabilistic realisability of channel transposition on finite dimensional systems with and without replicas.

Supermaps are attracting growing attentions in quantum computer science [30, 31, 32, 33] after a framework to analyse them was developed [34, 35, 36]. Supermaps have distinct properties that are not shared with usual maps, and much remains unexplored. For example, the optimal approximation of replication of unitary transformations behaves differently to the optimal approximation of state cloning [37]. Our analysis on state and channel transpositions offers a new perspective on the difference between maps and supermaps.

Besides of its fundamental interest, investigation on the required number of clones and replicas for state and channel transposition is important from a practical viewpoint. It is shown that simulation [38] or realisation [39] of state and channel transposition helps computation of several entanglement measures (see Sec. 2.3.4 for details). An already existing method [40] uses the classical description of the states and channels to simulate or realise transposition. If the description of the input state and map is not provided in advance, we have to perform tomography with sufficiently many state clones and map replicas. If there exists a method to realise the state and channel transposition without recourse to tomography, it might reduce the resource required for computing entanglement measures.

Generalising classical probability theory with topos quantum theory Topos quantum theory provides a method to represent quantum states as a direct generalisation of classical probability distributions formulated in the language of toposes. Toposes are special categories with a standard prescription to interpret a class of mathematical language (see Appx. C.4.2 for details). Category **Sets** of sets and functions is an example of topos, whose interpretation of the language corresponds to the usual set-theoretic logic. When a mathematical concept is interpreted in several toposes, they may have different properties. Real numbers and commutative C*-algebras can be formally defined by the mathematical language, and topos quantum theory uses their interpretation in certain toposes. If the mathematical concepts are interpreted in a topos, it is said to be internal to the topos.

Probability distributions are assignments of probability weights on the opens of topological space of random variables. In topos quantum theory, the topological space of random variables and probability distributions are generalised to *locales* and *valuations*, respectively. Valuations are probability weight assignments on locales. Topos quantum theory usually start from finding a suitable topos for a given Hilbert space or C*-algebra representing the quantum system of interest. Then an internal locale is constructed so that there exists a bijective correspondence between quantum states on the original system and valuations on the locale.

There is a large difference between locales describing classical probabilities and quantum states. The internal locales for representing quantum states do not usually have points, while the spaces of random variables always do (see, e.g. [41] for the definition of points on locales). Points of the locale, if exist, reveal non-contextual value assignments to physical observables, which is shown impossible for quantum theory by Kochen-Specker theorem [42]. Pointless locales can be used as quantum version of random variables to avoid contradiction to the Kochen-Specker theorem.

There are several other methods to represent quantum states by generalisations of probability distributions, such as quasi-probability distributions on phase spaces [43, 44] and Gleason's measure [45]. If we have a representation of quantum states by a generalised probability distribution, and if there is a proper definition of maps in the representation, we can ask how the difference between positive and CP maps emerges in that representation. For quasi-probability distributions, there is a generalised concept of transition matrices, i.e. classical positive maps [44], and it is capable of representing any linear maps. Thus the gap between positive and CP maps appears as well as usual quantum theory. As far as we know, there is no known canonical definition of maps between Gleason measures. For topos quantum theory, there is a straightforward method to generalise classical positive maps, to maps between valuations by using category theory (see Sec. 1.3.4 and Chap. 6 for details). It is not known, however, what the resulting maps represent, and we choose to investigate this problem.

Before proceeding to investigate maps between valuations, an appropriate definition of states on composite systems is required since the difference between positive and CP maps appears especially on composite systems. There are analyses on independence conditions of local systems in topos quantum theory [46, 47], and one can find a candidate of composite systems in Ref. [47] although their motivation is different from defining composite systems. Contrary to the composite systems, there is no analysis on valuations therein.

In our second approach, we first analyse correspondence between quantum states and valuations on composite systems. Since the composition of random variables is product, we define composite systems in topos quantum theory as product locales by employing and reinforcing results from [47]. Then we analyse the valuations on composite locales by using the several known theorems from constructive mathematics [48, 49]. Although there are bijective correspondence between quantum states on a Hilbert space and valuations on corresponding locales in a single system level, it is not guaranteed to be extended to our composite system.

Representation of valuations are relatively clear since they corresponds to points of a certain locale, whose formal definition is well known [49]. The analogous technique for transformations on valuations is not developed, and their explicit representation for topos quantum theory is not known. The lack of appropriate tools complicates the analysis of maps between valuations.

Instead of a direct analysis on maps between valuations, we consider generalisation of classical Markov chains to topos quantum theory. Markov chains in classical probability theory are particular kind of joint probability distributions on composite systems [50]. Classical Markov processes have already been generalised to quantum theory in several ways. In the context of open system dynamics, quantum Markov *processes* are those dynamics without recurrence of the system's information from the bath [12, 51, 52]. In the context of quantum information theory, quantum Markov *states* are those lacking a certain quantum correlation [53, 54].[2] Classical Markov chains, quantum Markov processes and quantum Markov states share a property that long Markov chains are constructed from short Markov ones by extending the latter with certain maps. Classical positive maps are used for extending classical Markov chains, CP [51] or positive maps [12] for quantum Markov processes, and CP maps for quantum Markov states [56]. In any cases, Markov chains reflect properties of maps from which they are constructed.

In this thesis, we generalise Markov chains to topos quantum theory. Markov chains thus defined are certain valuations on composite locales constructed from consecutive action of maps between valuations, and thus reflect properties of these maps. We analyse what kind of states on composite quantum systems, these generalised Markov chains correspond to. Since Markov chains are valuations, its analysis is more tractable than the maps between valuations themselves.

This thesis is organised as follows. In the remainder of this chapter, we give mathematical preliminaries for quantum theory and classical probability theory. The definitions of positive maps, CP maps, and corresponding supermaps are reviewed here. The definition and properties of classical Markov chains are also reviewed, and we reformulate in a category theoretical manner. In Chap. 2, we provide a review on positive non-CP maps, corresponding supermaps, and their use in quantum information science.

The original contribution of the present thesis begins from Chap. 3 and ends in Chap. 6. In the former two chapters, we investigate the relation between positive non-CP maps and non-linearity. In the latter two, we analyse composite systems and Markov chains in topos quantum theory.

In Chap. 3, we analyse probabilistic realisability of positive non-CP maps from finite clones. We show that transposition and certain class of positive non-CP maps require infinite number of clones. In Chap. 4, we turn to the probabilistic

[2] There are other generalisations of classical Markov chains not listed here. See [55], for example.

realisability of a particular positive non-CP supermap, namely channel transposition. We place special attention to channel transposition on unitary channels, and show an impossibility of channel transposition without replicas, and its possibility with replicas. We also show an application of channel transposition to compute entanglement measures.

At the beginning of Chap. 5, we give a more detailed introduction to topos quantum theory. Then in the remainder of that chapter, we investigate valuations on composite systems in topos quantum theory. We show a bijective correspondence between positive over pure tensor states and valuations on our composite systems. Based on this result, we define Markov chains in topos quantum theory, and analyse their properties in Chap. 6. We analyse a monogamy property of positive over pure tensor states independently to toposes, and show that our definition of Markov chains in topos quantum theory leads to trivial valuations by applying the monogamy property.

Finally we lay our conclusion with some open problems in Chap. 7.

1.1 Quantum maps

We start from a review on basic definitions and physical meanings of maps on quantum states. We introduce operators and maps on Hilbert spaces, and notations used throughout this thesis in Sec. 1.1.1. Physical meanings of these mathematical concepts required for understanding Chap. 3 and Chap. 4 are introduced in Sec. 1.1.2.

We only consider Hilbert spaces with finite dimensions in this thesis. For representing vectors of Hilbert space and their dual, we use the "ket" $|\psi\rangle$ and "bra" $\langle\phi|$, so that the inner product is denoted by $\langle\phi|\psi\rangle$. We use $*$ to denote complex conjugation on scalars and operators in the computational basis, and $\dagger$ to denote the Hermitian adjoint.

1.1.1 Mathematical definitions

We review operators and maps on Hilbert spaces. Precise definitions of positive and CP maps, which are our main concern in this thesis, are given in this section.

Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces. Unit vectors of $\mathcal{H}$ are called pure state vectors. We denote the set of bounded linear operators from $\mathcal{H}$ to $\mathcal{K}$ by $\mathcal{B}(\mathcal{H},\mathcal{K})$, and in particular by $\mathcal{B}(\mathcal{H})$ if the output space $\mathcal{K}$ is equal to the input $\mathcal{H}$. A linear operator O on $\mathcal{H}$ is called unitary if $O^\dagger O$ and $OO^\dagger$ coincide with the identity operator $\mathbb{I}$, and Hermitian if $O = O^\dagger$. We denote the set of Hermitian operators on $\mathcal{H}$ by $\mathcal{B}(\mathcal{H})_{\mathrm{sa}}$ with "sa" for self-adjoint.

A linear operator Π satisfying $\Pi = \Pi^\dagger = \Pi^2$ is called an projector. A projector Π is decomposable into $\Pi = \sum_i^n |\psi_i\rangle\langle\psi_i|$ with some set of orthogonal pure state vectors $\{|\psi_i\rangle\}$, and the integer n is called the rank of projector Π. An operator O on $\mathcal{H}$ is called positive semi-definite if it is Hermitian and its eigenvalues are all non-negative. Equivalently, O is positive semi-definite if

$$\mathrm{Tr}[O\Pi] \geq 0 \tag{1.1}$$

for any projectors on $\mathcal{H}$, where $\mathrm{Tr}[\cdot]$ represents the trace. The set of positive semi-definite operators on $\mathcal{H}$ is denoted by $\mathrm{Pos}(\mathcal{H})$. A partial ordering $\leq$ between operators on $\mathcal{H}$ is defined by

$$O_1 \leq O_2 \ \Leftrightarrow\ O_2 - O_1 \in \mathrm{Pos}(\mathcal{H}). \tag{1.2}$$

Positive semi-definite operators ρ with unit trace $\mathrm{Tr}[\rho] = 1$ are called density operators. The set of density operators on $\mathcal{H}$ is denoted by $\mathcal{S}(\mathcal{H})$, and we call it the state space on $\mathcal{H}$. The state space $\mathcal{S}(\mathcal{H})$ is convex and includes pure states $|\psi\rangle\langle\psi|$ as the extremal points.

A linear map from $\mathcal{B}(\mathcal{H})$ to $\mathcal{B}(\mathcal{K})$ is called Hermitian preserving if it maps all Hermitian operators in $\mathcal{B}(\mathcal{H})$ to those in $\mathcal{B}(\mathcal{K})$, and *positive* if it maps all positive semi-definite operators in $\mathcal{B}(\mathcal{H})$ to those in $\mathcal{B}(\mathcal{K})$. If a positive map $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ further satisfies

$$\mathrm{id}_{\mathbb{C}_k} \otimes \mathcal{E}(O) \geq 0 \qquad (\forall O \in \mathrm{Pos}(\mathbb{C}_k \otimes \mathcal{H})) \tag{1.3}$$

with k dimensional Hilbert space $\mathbb{C}_k$, then it is called k-positive. Here $\mathrm{id}_{\mathcal{H}}$ represents the identity map on $\mathcal{B}(\mathcal{H})$. If a positive map is k-positive, then it is k'-positive for all k' smaller than k. If a positive map $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ is $(\dim \mathcal{H})$-positive, then it is known to be k-positive for any larger k, and called *completely positive* (CP). The set of all CP maps from $\mathcal{B}(\mathcal{H})$ to $\mathcal{B}(\mathcal{K})$ is denoted by $\mathrm{CP}(\mathcal{B}(\mathcal{H}), \mathcal{B}(\mathcal{K}))$. A linear map $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ is called trace preserving (TP) if it satisfies

$$\mathrm{Tr}[\mathcal{E}(\rho)] = 1 \ (\forall \rho \in \mathcal{S}(\mathcal{H})), \tag{1.4}$$

and trace non-increasing (TNI) if

$$\mathrm{Tr}[\mathcal{E}(\rho)] \leq 1 \ (\forall \rho \in \mathcal{S}(\mathcal{H})). \tag{1.5}$$

An *instrument* is a set $\{\mathcal{E}_i : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})\}_{i=1,\ldots,n}$ of TNICP maps such that $\sum_{i=1}^n \mathcal{E}_i$ is a TPCP map.

Transposition is an example of TP positive map that is not CP. Transposition is a linear map that transposes given operators in terms of a fixed basis. Throughout this thesis, we denote the transposition of interest by T $(: \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}))$ and the basis of transposition by $\{|i\rangle\}_{i=1,\ldots,\dim \mathcal{H}}$ called the computational basis. For example, the transposition of $|i\rangle\langle j|$ is $|j\rangle\langle i|$.

If operator O is a linear (or antilinear) operator from $\mathcal{H}$ to $\mathcal{K}$, $\mathcal{U}[O] : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ denotes O's adjoint action on operators on $\mathcal{H}$:

$$\mathcal{U}[O](A) := OAO^\dagger.$$

If U is a unitary operator, the adjoint action $\mathcal{U}[U]$ is a TPCP map which is called a unitary channel.

1.1.2 Quantum theory and implementation of completely positive maps

In this subsection, we introduce the notion of quantum systems, and physical meanings of linear maps introduced in the previous subsection. A quantum system in this thesis refers to any physical objects whose state is described by a density operator on a Hilbert space. The standard quantum physics stipulates that the state of a closed quantum system evolves according to a unitary channel. However, the classes of states a physical object may take varies according to, for instance, how they are composed to each other and how the part of systems are described. In this thesis, we take an abstract formulation of quantum systems which does not rely on the actual physical object like photons, electrons in the shell, etc.... This formulation is widely used in quantum information theory, and we call this *quantum theory*.

If a quantum system is described by $\mathcal{H}$, the system may take any density operators in $\mathcal{S}(\mathcal{H})$ as a state. All the self adjoint operators on $\mathcal{H}$ are observables whose expectation values can be estimated by quantum measurements defined later. If there are two quantum systems described by the Hilbert spaces $\mathcal{H}$ and $\mathcal{K}$, their composite system is described by the tensor product Hilbert space $\mathcal{H} \otimes \mathcal{K}$. If the state of composite system is $\rho \in \mathcal{S}(\mathcal{H} \otimes \mathcal{K})$, its marginal state on $\mathcal{H}$ is defined by the partial trace $\mathrm{Tr}_\mathcal{K}[\rho]$ so that

$$\mathrm{Tr}[A \mathrm{Tr}_\mathcal{K}[\rho]] = \mathrm{Tr}[(A \otimes \mathbb{I}_\mathcal{K})\rho] \ (\forall A \in \mathcal{B}(\mathcal{H})). \tag{1.6}$$

We do not consider the additional rules such as superselection.

In Chaps. 3 and 4, we consider physical realisability of certain maps and supermaps defined in Sec. 1.2. The realisability is determined by what we can do on quantum systems. When we try to manipulate quantum systems, we assume the existence of machines which we call *quantum manipulators*. Quantum manipulators are assumed to be capable of implementing any instruments to the systems of interest. When we implement instrument $\{\mathcal{E}_i : \mathcal{H}_1 \to \mathcal{H}_2\}_i$ on (potentially) a part of the composite quantum system $\mathcal{H}_1 \otimes \mathcal{K}$ whose state is $\rho \in \mathcal{S}(\mathcal{H}_1 \otimes \mathcal{K})$, we obtain the state

$$\frac{\mathcal{E}_i \otimes \mathrm{id}_{\mathcal{K}}(\rho)}{p_i(\rho)} \tag{1.7}$$

with probability

$$p_i(\rho) := \mathrm{Tr}[\mathcal{E}_i \otimes \mathrm{id}_{\mathcal{K}}(\rho)] = \mathrm{Tr}[\mathcal{E}_i(\mathrm{Tr}_{\mathcal{K}}[\rho])], \tag{1.8}$$

and with an outcome of classical information of index i the state is transformed according to TNICP map $\mathcal{E}_i$, among the set $\{\mathcal{E}_i\}$.

We sometimes consider applying instruments on (potentially cloned) quantum states uncorrelated to other systems. A bipartite quantum state $\rho \in \mathcal{S}(\mathcal{H}_1 \otimes \mathcal{K})$ is said to be uncorrelated if it is a product $\rho_{\mathcal{H}_1} \otimes \rho_{\mathcal{K}}$ of states $\rho_{\mathcal{H}_1} \in \mathcal{S}(\mathcal{H}_1)$ and $\rho_{\mathcal{K}} \in \mathcal{S}(\mathcal{K})$. A state $\rho \in \mathcal{S}(\mathcal{H}_1)$ is said to be *uncorrelated to other systems* or just *uncorrelated* if one does not have accessibility to the other system $\mathcal{K}$ on which ρ is a marginal state of a correlated bipartite state $\rho_{\mathcal{H}_1 \otimes \mathcal{K}} \in \mathcal{S}(\mathcal{H}_1 \otimes \mathcal{K})$. An instrument $\{\mathcal{E}_i : \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{H}_2)\}$, applied on the state $\rho \in \mathcal{S}(\mathcal{H}_1)$ uncorrelated to other systems, produces the state

$$\frac{\mathcal{E}_i(\rho)}{p_i(\rho)}, \tag{1.9}$$

with probability $p_i(\rho) = \mathrm{Tr}[\mathcal{E}_i(\rho)]$.

Instruments are closed under composition. If we have two quantum manipulators implementing instruments $\{\mathcal{E}^1_i : \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{K}_1)\}$ and $\{\mathcal{E}^2_j : \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{K}_2)\}$ respectively, the set $\{\mathcal{E}^1_i \otimes \mathcal{E}^2_j : \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2) \to \mathcal{B}(\mathcal{K}_1 \otimes \mathcal{K}_2)\}$ defines an instrument. If we implement instruments $\{\mathcal{E}^1_i : \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{H}_2)\}$ and $\{\mathcal{E}^2_i : \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_3)\}$ in a sequence, it is equivalent to implementing an instrument $\{\mathcal{E}^2_j \circ \mathcal{E}^1_i : \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{H}_3)\}$. Spatial and temporal composition of quantum manipulators constitute a single large quantum manipulator.

TPCP maps are instruments consisting of only 1 component of the CP map, and said to be *deterministically realisable* because quantum manipulators can implement the map with unit probability. TNICP maps are said to be *probabilistically realisable* because for any TNICP map $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$, there is another TNICP map $\mathcal{E}' : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ such that $\{\mathcal{E}, \mathcal{E}'\}$ is an instrument, and thus $\mathcal{E}$ can be implemented with some probability (see footnote 1 in Chap. 2 for an explicit construction of $\mathcal{E}'$ from $\mathcal{E}$). Examples of TPCP maps are unitary channels $\mathcal{U}[U]$ and state preparations $\rho : \mathcal{B}(\mathbb{C}) \to \mathcal{B}(\mathcal{H})$ to generate a state ρ in the system $\mathcal{H}$. An example of TNICP map is measurements followed by post-selection. A quantum measurement on $\mathcal{H}$ is described by a set of measurement operators $\{M_i\}$ on $\mathcal{H}$

such that $\sum_i M_i^\dagger M_i = \mathbb{I}_\mathcal{H}$, and its action on states is the instrument $\{\mathcal{U}[M_i]\}$ where i represents the outcome of measurement. The measurement followed by post-selection means to select each component $\mathcal{U}[M_i]$.

When we consider realisability of certain maps and supermaps in Chaps. 3 and 4 with quantum manipulators, we do not care the actual experimental procedures that quantum manipulators take when they implement instruments. Still it would be worth commenting that combinations of a limited sorts of quantum manipulators is sufficient to express any instruments. It is known that any instrument decomposes into preparation of an ancillary state, a unitary channel, and quantum measurements. More precisely, a set of linear maps $\{\mathcal{E}_i : \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{H}_2)\}$ is an instrument if and only if it is expressed by

$$\mathcal{E}_i(\rho) = \mathrm{Tr}_{\mathcal{H}_1 \otimes \mathcal{K}} \left[(\mathbb{I}_{\mathcal{H}_1 \otimes \mathcal{H}_2} \otimes \Pi_i) U (\rho \otimes \rho_0) U^\dagger (\mathbb{I}_{\mathcal{H}_1 \otimes \mathcal{H}_2} \otimes \Pi_i) \right], \tag{1.10}$$

with a Hilbert space $\mathcal{K}$, a state $\rho_0 \in \mathcal{S}(\mathcal{H}_2 \otimes \mathcal{K})$, projectors Π_i such that $\sum_i \Pi_i = \mathbb{I}_\mathcal{K}$, and a unitary operator U on $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{K}$ [57, 58]. Quantum measurements are said to be projective if the measurement operators are projectors. Thus if state preparation, arbitrary unitary transformations, and arbitrary projective measurements are all realisable with certain experimental procedure, any instrument can be realised by combining these elements.

In Sec. 4.3, we consider observables to measure certain quantities such as entanglement. Expectation values of observables can be calculated from the outcome statistics of corresponding measurements. For calculating the expectation value $\mathrm{Tr}[A\rho]$ of observable A for the state $\rho \in (\mathcal{H})$, find a set of measurement operators $\{M_i\}$ such that $A = \sum_i a_i M_i^\dagger M_i$ where each a_i is a real number. The expectation value is expressed in terms of the probabilities p_i to obtain outcomes i by

$$\mathrm{Tr}[A\rho] = \sum_i a_i \mathrm{Tr}[M_i^\dagger M_i \rho] = \sum_i a_i \mathrm{Tr}[\mathcal{U}[M_i](\rho)] = \sum_i a_i p_i. \tag{1.11}$$

A standard choice of the measurement operators would be $M_i = |\psi_i\rangle\langle\psi_i|$ with A's spectral decomposition $A = \sum_i a_i |\psi_i\rangle\langle\psi_i|$. If we implement the measurement on infinitely many clones of the state ρ, we would obtain the probability distribution of $\{p_i\}$, and hence the expectation value.

It is possible to determine the description of quantum states from outcome probabilities of a set of measurements called informationally complete measurements. The procedure for determining the description of a given state in experiments is called *state tomography*. Since the observed finite outcome probabilities of measurements are not necessary to be the exact probability distribution, state tomography never reaches to the exact description of states in the real experiment. In this thesis, we consider an ideal situation where the gap between the observed distribution and the exact distribution does not exist. In this case, a set of measurement performed on infinite clones of the unknown state is sufficient to obtain the exact outcome probabilities, from which the exact description of the state is calculated (see Appx. A for example).

1.2 Supermaps

As a part of our first approach to connect quantum theory and classical probability theory, we analyse realisability of a positive non-CP *supermap* with added non-linearity in Chap. 4. A supermap here refers to a map whose input and output is already a map representing a state transformation. In this thesis, we focus on supermaps whose inputs are (potentially replicated) TPCP maps and outputs are CP maps. Thus mathematically, a supermap f is a map from $\mathrm{CP}(\mathcal{B}(\mathcal{H}), \mathcal{B}(\mathcal{K}))$ to $\mathrm{CP}(\mathcal{B}(\mathcal{H}'), \mathcal{B}(\mathcal{K}'))$ if the domain and codomain of the input TPCP maps are $\mathcal{H}$ and $\mathcal{K}$ respectively, and if those of the output CP maps are $\mathcal{H}'$ and $\mathcal{K}'$ respectively. Here we give a definition of realisable supermaps in Sec. 1.2.1 and review a supermap formalism presented in Refs. [34, 35, 36] in Sec. 2.2.2. We define positive and CP supermaps based on the reviewed framework. One can skip this section if not interested in our investigation on channel transposition presented in Chap. 4.

1.2.1 Realisability of supermaps

When we considered the implementability of TNICP maps and TPCP maps in Sec. 1.1.2, inputs and outputs of the map are both states. This class of map should be called realisable if there exists an instrument that outputs desired states depending on the input states. Behind this definition, we assume the existence of a physical devise called “source” that generates one of the states on a fixed Hilbert space. We try to make the desired output by using a quantum manipulator *after* the state is generated.

On the other hand, the input of a supermap is an unknown TPCP map. We assume that in a certain period of time, a physical devise suffers an unknown state transformation represented by a TPCP map, say, $\Gamma : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$. We try to construct another devise which implements TPCP map $f(\Gamma) : \mathcal{B}(\mathcal{H}') \to \mathcal{B}(\mathcal{K}')$ by using this devise and a quantum manipulator. Unlike the case of state transposition, we are able to use the quantum manipulator in three different steps: forward processing before the unknown transformation happens, side processing running in parallel to the state transformations and the post processing after the state transformation (see Fig. 1.2 (a)). The quantum manipulator with these three steps is described by two CP maps $\mathcal{E} : \mathcal{B}(\mathcal{H}') \to \mathcal{B}(\mathcal{H} \otimes \mathcal{H}_A)$ and $\mathcal{D} : \mathcal{B}(\mathcal{K} \otimes \mathcal{H}_A) \to \mathcal{B}(\mathcal{K}')$ called encoder and decoder, respectively. A devise implementing

$$\mathcal{D} \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \Gamma) \circ \mathcal{E} \tag{1.12}$$

is constructed by using the quantum manipulator and the input devise (see Fig. 1.2 (b)). The forward and post processing are included in the encoder $\mathcal{E}$ and the decoder $\mathcal{D}$ respectively, and the side processing is included in either of them. The ancillary Hilbert space $\mathcal{H}_A$ represents a quantum memory. We say that a supermap $\Gamma \mapsto f(\Gamma)$ is probabilistically (deterministically) realisable if there is a pair of TNICP (TPCP) maps $\mathcal{E}$ and $\mathcal{D}$, such that Eq. (1.12) represents $f(\Gamma)$ (we shall give precise definitions for each individual problem).

We also consider a supermap whose input is replicated TPCP maps. Imagine a devise whose state suffers collective action $\Gamma^{\otimes m}$ of a TPCP map Γ. We wish to make another devise which implements $f(\Gamma)$ by using this device and a quantum

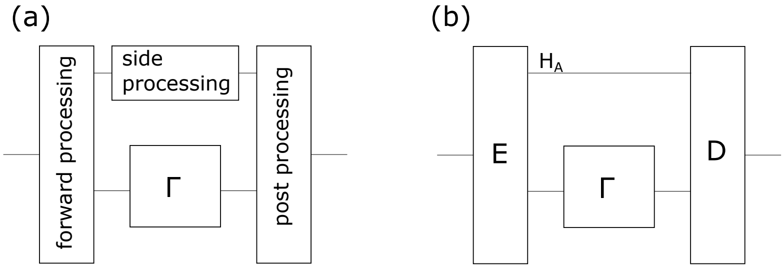

Figure 1.2: Two equivalent quantum circuits to realise a supermap. (a) A quantum circuit representing a strategy to realise a supermap. Quantum manipulators implement CP maps before, after, and during the unknown TPCP map. In other words, the unknown TPCP map is given as an oracle. (b) A quantum circuit representing the same CP map presented by (a). The side processing appearing in (a) is merged to either forward or post processing, and the circuit reduces to two components called encoder (labelled E) and decoder (labelled D).

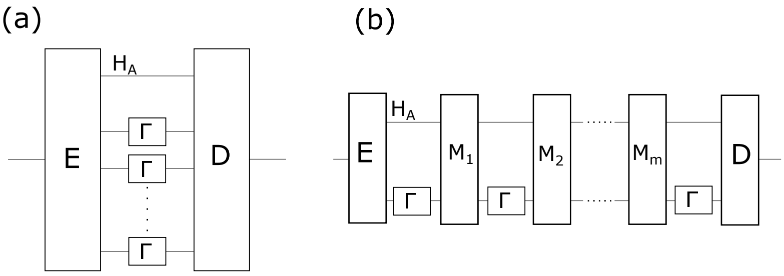

Figure 1.3: General strategies to realise a supermap when the replicas of unknown TPCP map Γ is given (a) in parallel, and (b) in a sequence.

manipulator. In this case, the realisable supermaps are defined just by replacing Γ to $\Gamma^{\otimes m}$ in Eq. (1.12):

$$\mathcal{D} \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \Gamma^{\otimes m}) \circ \mathcal{E}, \tag{1.13}$$

where the domain of $\mathcal{D}$ and the codomain of $\mathcal{E}$ should be set accordingly (see Fig. 1.3 (a)). In a more general situation, the replicas of Γ may be given sequentially. For example, if a devise evolves according to Hamiltonian dynamics $\exp(-iHt)$ and if a quantum manipulator may interfere the devise at every Δt intervals, we are given replicas of $\exp(-iH\Delta t)$ in a sequence. In this case we can perform quantum computation in each interval after a Hamiltonian dynamics finishes and before the next one starts. In this way, we can construct a devise implementing

$$\mathcal{D} \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \Gamma) \circ \mathcal{M}_{m-1} \circ \ldots \circ \mathcal{M}_2 \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \Gamma) \circ \mathcal{M}_1 \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \Gamma) \circ \mathcal{E}, \tag{1.14}$$

where $\mathcal{E}$ and $\mathcal{D}$ are the encoder and the decoder, and $\mathcal{M}_i : \mathcal{B}(\mathcal{K} \otimes \mathcal{H}_A) \to \mathcal{B}(\mathcal{H} \otimes \mathcal{H}_A)$ in the middle are CP maps (see Fig. 1.3 (b)). The realisable supermaps from sequentially given replicas are defined analogously.

If a supermap is realisable from replicas given in parallel, then it is also realisable from a sequentially given replicas. If we set $\mathcal{E}$, $\mathcal{D}$, and $\mathcal{M}_i$'s carefully,

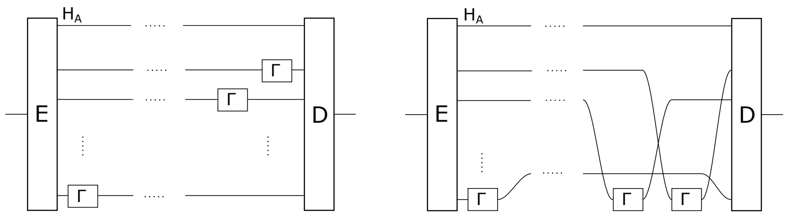

Figure 1.4: Quantum circuits to simulate replicas given in parallel by sequentially given ones. These quantum circuits represent a CP map equivalent to the one represented by Fig. 1.3 (a).

Eq. (1.14) reduces to Eq. (1.13). See Fig. 1.4 for details of this observation. Replicas of TPCP maps given in a sequence are the most powerful in this sense.

Remark 1. Note that the device constructed by Eqs. (1.12), (1.13) and (1.14) have a restriction on the timing to be used. The devise must obtain input states before the unknown state transformation happens in the original devise. This is in contrast to *quantum learning* investigated in Ref. [59], where the desired TPCP maps are implemented after the original TPCP map finishes.

1.2.2 Positive and CP supermaps

In the previous subsection we have seen that a realisable supermap from a single unknown TPCP map is characterised by the pair of CP maps called encoder and decoder. An alternative characterisation is provided and shown to be equivalent to the one by the encoder and the decoder [34, 35, 36]. We define positive and CP supermaps by using the technique presented there. Although this alternative characterisation is extensible to realisable supermaps from replicated TPCP maps [35, 36], we only review the case without replication since this suffice for our purpose.

The following representation of linear maps is frequently used in Chap. 4 mainly in the analysis on supermaps, but also for other purposes. Define a linear map χ from linear maps in $\mathcal{B}(\mathcal{B}(\mathcal{H}), \mathcal{B}(\mathcal{K}))$ to operators in $\mathcal{B}(\mathcal{H} \otimes \mathcal{K})$ by

$$\chi(\mathcal{E}) := \mathrm{id}_{\mathcal{H}} \otimes \mathcal{E}(\Phi_{\mathcal{H},\mathcal{H}}), \tag{1.15}$$

for all $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$, where $\Phi_{\mathcal{H},\mathcal{H}} := \sum_{i,j=1}^{\dim \mathcal{H}} |i, i\rangle\langle j, j|$. The map χ is bijective and its inverse χ^{-1} is given by

$$\chi^{-1}(C)(A) := \mathrm{Tr}_{\mathcal{H}}[C A^{\mathrm{T}}] \quad (\forall A \in \mathcal{B}(\mathcal{H})), \tag{1.16}$$

for all $C \in \mathcal{B}(\mathcal{H} \otimes \mathcal{K})$. This bijection is restricted to the map-operator correspondence presented in Table 1.1. The map χ is called the Choi isomorphism, and $\chi(\mathcal{E})$ is called the Choi operator for $\mathcal{E}$, and we denote it by $\widetilde{\mathcal{E}}$ in this thesis. The Choi isomorphism reduces maps into operators, and as we shall review in the following, it reduces supermaps into maps.

Let us consider a supermap f from TPCP maps in $\mathrm{CP}(\mathcal{B}(\mathcal{H}_1), \mathcal{B}(\mathcal{K}_1))$ to those in $\mathrm{CP}(\mathcal{B}(\mathcal{H}_2), \mathcal{B}(\mathcal{K}_2))$. Since the Choi isomorphism χ provides a bijective correspondence between CP maps and bipartite positive operators, the supermap can

map $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$	operator $\widetilde{\mathcal{E}} \in \mathcal{B}(\mathcal{H} \otimes \mathcal{K})$
Hermitian preserving	Hermitian
Positive	1-positive
CP	positive semi-definite

Table 1.1: The map-operator correspondence provided by the Choi isomorphism. 1-positive operator refers to any operator $\omega \in \mathcal{B}(\mathcal{H} \otimes \mathcal{K})$ such that $\mathrm{Tr}[\omega(|\psi\rangle\langle\psi| \otimes |\phi\rangle\langle\phi|)] \geq 0$ for any pair of quantum states $|\psi\rangle$ on $\mathcal{H}$ and $|\phi\rangle$ on $\mathcal{K}$ (See Sec. 2.1.1 for more details).

be equivalently well represented by a composition

$$\begin{aligned} \mathscr{S}_f \quad : \quad & \mathrm{Pos}(\mathcal{H}_1 \otimes \mathcal{K}_1) \xrightarrow{\chi^{-1}} \mathrm{CP}(\mathcal{B}(\mathcal{H}_1), \mathcal{B}(\mathcal{K}_1)) \\ & \xrightarrow{f} \mathrm{CP}(\mathcal{B}(\mathcal{H}_2), \mathcal{B}(\mathcal{K}_2)) \xrightarrow{\chi} \mathrm{Pos}(\mathcal{H}_2 \otimes \mathcal{K}_2). \end{aligned}$$

From $\mathscr{S}_f$, f is recovered by the inverse transformation

$$\begin{aligned} f \quad : \quad & \mathrm{CP}(\mathcal{B}(\mathcal{H}_1), \mathcal{B}(\mathcal{K}_1)) \xrightarrow{\chi} \mathrm{Pos}(\mathcal{H}_1 \otimes \mathcal{K}_1) \\ & \xrightarrow{\mathscr{S}_f} \mathrm{Pos}(\mathcal{H}_2 \otimes \mathcal{K}_2) \xrightarrow{\chi^{-1}} \mathrm{CP}(\mathcal{B}(\mathcal{H}_2), \mathcal{B}(\mathcal{K}_2)). \end{aligned}$$

The necessary and sufficient condition on map $\mathscr{S} : \mathrm{Pos}(\mathcal{H}_1 \otimes \mathcal{K}_1) \to \mathrm{Pos}(\mathcal{H}_2 \otimes \mathcal{K}_2)$ to correspond to a realisable supermap f is derived in Refs. [34, 35, 36]. We rewrite the condition in a way convenient for our use.

Lemma 2 ([36])**.** Let $f_{\mathscr{S}}$ be a supermap defined by $\mathscr{S} : \mathrm{Pos}(\mathcal{H}_1 \otimes \mathcal{K}_1) \to \mathrm{Pos}(\mathcal{H}_2 \otimes \mathcal{K}_2)$ via Eq. (1.17). There exists a pair of TP encoder $\mathcal{E} : \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_A)$ and decoder $\mathcal{D} : \mathcal{B}(\mathcal{K}_1 \otimes \mathcal{H}_A) \to \mathcal{B}(\mathcal{K}_2)$ such that

$$f_{\mathscr{S}}(\Gamma) = \mathcal{D} \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \Gamma) \circ \mathcal{E} \tag{1.17}$$

for any Γ if and only if (i) $\mathscr{S}$ is a CP map, and (ii) $\mathrm{Tr}_{\mathcal{K}_2}[\widetilde{\mathscr{S}}] = \mathbb{I}_{\mathcal{K}_1} \otimes \widetilde{\mathscr{S}'}$, where $\widetilde{\mathscr{S}'}$ is the Choi matrix of a TPCP map $\mathscr{S}' : \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_1)$. There exists a pair of TNI encoder $\mathcal{E} : \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_A)$ and decoder $\mathcal{D} : \mathcal{B}(\mathcal{K}_1 \otimes \mathcal{H}_A) \to \mathcal{B}(\mathcal{K}_2)$ such that

$$f_{\mathscr{S}}(\Gamma) \propto \mathcal{D} \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \Gamma) \circ \mathcal{E} \tag{1.18}$$

for any Γ if and only if (i) holds and (iii) $\widetilde{\mathscr{S}} \leq \widetilde{\mathscr{S}''}$ for some $\mathscr{S}'' : \mathrm{Pos}(\mathcal{H}_1 \otimes \mathcal{K}_1) \to \mathrm{Pos}(\mathcal{H}_2 \otimes \mathcal{K}_2)$ satisfying (i) and (ii).

We use Lem. 2 for proving a no-go theorem of unitary conjugation in Sec. 4.2.1 (we only use the condition (i) for this purpose).

Now we can define positive and CP supermaps as in the case of maps as mentioned in the introduction. We call a supermap f to be *positive* if $\mathscr{S}_f$ is a positive map and satisfies the condition (iii) of Lem. 2. If $\mathscr{S}_f$ is further CP, we call f to be *completely positive* (CP). Lemma 2 states that CP supermaps are realisable by appropriate pairs of encoders and decoders.

The input maps of the positive non-CP supermaps must be disentangled to other systems so that the outputs of the supermaps to be valid quantum maps. Let $\widetilde{\Gamma} \in \mathrm{Pos}(\mathcal{H}_1 \otimes \mathcal{H}_1{}' \otimes \mathcal{K}_1 \otimes \mathcal{K}_1{}')$ be the Choi operator of a TPCP map $\Gamma : \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_1{}') \to \mathcal{B}(\mathcal{K}_1 \otimes \mathcal{K}_1{}')$, and $\mathscr{S}_f : \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{K}_1) \to \mathcal{B}(\mathcal{H}_2 \otimes \mathcal{K}_2)$ be a map corresponding to a positive non-CP supermap $f : \mathrm{CP}(\mathcal{B}(\mathcal{H}_1), \mathcal{B}(\mathcal{K}_1)) \to \mathrm{CP}(\mathcal{B}(\mathcal{H}_2), \mathcal{B}(\mathcal{K}_2))$. The action of f applied only on a part of the multi-party TPCP map Γ produces a multi-party map whose Choi operator is given by

$$\mathscr{S}_f \otimes \mathrm{id}_{\mathcal{H}_1{}' \otimes \mathcal{K}_1{}'}(\widetilde{\Gamma}).$$

This operator does not necessarily represent a multi-party CP map if $\widetilde{\Gamma}$ is entangled in the bi-partition $\mathcal{H}_1 \otimes \mathcal{K}_1$-$\mathcal{H}_1{}' \otimes \mathcal{K}_1{}'$, since the positive non-CP map $\mathscr{S}_f$ applied only on a part of the multi-party Choi operator may output a non-positive operator (see Sec. 2.1.1 for details). Thus positive non-CP supermaps are not valid transformations on maps when applied on a part of quantum systems. When we consider realisability of positive non-CP supermaps in Chap. 4, we assume that the input maps are uncorrelated to other systems in terms of the Choi operator representation, in order to avoid the impossiblity implied by the non-validity of supermaps.

1.3 Representation of classical probaiblity distributions and maps

In this section, we revisit the definition of probability distribution, transition matrices and Markov chains, and reformulate it category theoretically. This would be a preparation for generalising the Markov chains for topos quantum theory in Chap. 6. We start from reviewing the definition of classical probability distributions and transition matrices in Sec. 1.3.1. An equivalence between trantision matrices and classical positive maps is shown in Sec. 1.3.2, where we also give an introduction to C*-algebras used in Chap. 5. In Sec. 1.3.3, we review the definition of classical Markov chains. In the remaining subsections, we introduce a category theoretical definition of probability distributions, transition matrices, and Markov chains, which might be unfamiliar to physicists. Subsection 1.3.4 is devoted to definitions of monad and its Kleisli category. Finally in Sec. 1.3.5, we reformulate classical Markov chains in terms of distribution monad. We assume familiarity on notions from basic category theory presented in Appx. C.1 and Appx. C.2 to read Secs. 1.3.4 and 1.3.5.

1.3.1 Probability distributions and transition matrices

Classical probability theory deals with random variables with associated probability distributions. A random variable is a set. In this thesis, we assume that the set of random variables are all finite. If there are several random variables $X_1, ..., X_n$, the composite random variable is represented by the product set $X_1 \times ... \times X_n$.

A function $p : X \to [0, 1]$ on random variable X is called a probability distribution on X if $\sum_{x \in X} p(x) = 1$. Probability distributions on composite random variables are called joint probability distributions. If $p_{XY} : X \times Y \to [0,1]$ is a joint probability distribution, its marginal distribution $p_Y : Y \to [0,1]$ on Y is defined by

$$p_Y(y) = \sum_{x \in X} p_{XY}(x,y). \tag{1.19}$$

Conditional probability distribution $p_{X|Y}$ of p_{XY} conditioned on Y is defined by

$$p_{X|Y}(x|y) := \frac{p_{XY}(x,y)}{p_Y(y)}. \tag{1.20}$$

Transformations between probability distributions are represented by transition matrices. Transition matrix $[f(x)(y)]_{x \in X,\ y \in Y}$ from X to Y is a $|X|$-by-$|Y|$ matrix with entries $f(x)(y) \in [0,1]$ satisfying $\sum_y f(x)(y) = 1$ for all $x \in X$. If a transition matrix $[f(x)(y)]_{x \in X,\ y \in Y}$ from X to Y is applied on a probability distribution $p_X : X \to [0,1]$, we obtain a probability distribution

$$p_Y(y) := \sum_{x \in X} p_X(x) f(x)(y) \tag{1.21}$$

on Y.

Transition matrices are the classical version of positive maps. In the next subsection, we review the general definition of positive maps and equivalence of the classical version of positive maps to transition matrices.

1.3.2 Positive and CP maps on C*-algebras

The notions of positive and CP maps in classical probability theory and quantum theory are unified by introducing maps between C*-algebras. Here, we give an introduction to C*-algebras as a reparation to Chap. 5, and summarise the relation between maps of C*-algebras and maps of quantum and classical probability theory.

We first recall the definition of C*-algebras[3]. A unital C*-algebra is an algebra A with the unit of multiplication $\mathbb{I}$, a complex complete norm $||\cdot||$ and a conjugate linear involution $\dagger : A \to A$ such that for all $a, b \in A$ and $\lambda \in \mathbb{C}$,

$$\begin{aligned} ||ab|| &\leq ||a||\, ||b||, \\ (a+b)^\dagger &= a^\dagger + b^\dagger, \\ (\lambda a)^\dagger &= \lambda^* a^\dagger, \\ a^{\dagger\dagger} &= a, \\ (ab)^\dagger &= b^\dagger a^\dagger, \\ ||a^\dagger a|| &= ||a||^2. \end{aligned}$$

It is further called commutative, if $ab = ba$ holds for all $a, b \in A$.

[3]The C*-algebra presented here is internal to **Sets**. C*-algebras can be defined in a more formal manner. In Chap. 5, we interpret the formal definition in other toposes than **Sets**.

A bounded linear map $\mathcal{E} : A \to B$ between unital C*-algebras is said to be (i) unital if $\mathcal{E}(\mathbb{I}_A) = \mathcal{E}(\mathbb{I}_B)$, where $\mathbb{I}_A$ and $\mathbb{I}_B$ are the units, (ii) $*$-homomorphism, if for all $a, b \in A$,

$$\begin{aligned} \mathcal{E}(ab) &= \mathcal{E}(a)\mathcal{E}(b), \\ \mathcal{E}(a^\dagger) &= \mathcal{E}(a)^\dagger, \\ \mathcal{E}(\mathbb{I}_A) &= \mathcal{E}(\mathbb{I}_B) \end{aligned}$$

hold, and (iii) *positive* if

$$\mathcal{E}(a) \geq 0 \text{ whenever } a \geq 0$$

hold. The definition of complete positivity require a few more steps. If A is a C*-algebra $M_k(A)$ denotes the C*-algebra whose elements are $k \times k$-matrices with entries from A. The multiplication and summation of elements in $M_k(A)$ are defined by the matrix multiplication and summation. A bounded linear map $\mathcal{E} : A \to B$ is said to be *completely positive* if $M_k(f) : M_k(A) \to M_k(B)$, defined by $\mathcal{E}$ acting on each element, is positive for all $k \in \mathbb{N}$.

When $A = \mathcal{B}(\mathcal{H}_A)$ and $B = \mathcal{B}(\mathcal{H}_B)$ with finite dimensional Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, there is a bijective correspondence between positive (CP) maps from $\mathcal{B}(\mathcal{H}_B)$ to $\mathcal{B}(\mathcal{H}_A)$ introduced in Sec. 1.1.1 and positive (CP) maps of C*-algebras from A to B (note that the order of domain and codomain is exchanged). The bijection is given by taking dual in the Hilbert-Schmidt inner product spaces (see Appx. A for details), and TP maps are dual to unital maps of C*-algebras. This duality states the equivalence of the Schrodinger picture and the Heisenberg picture. In this way, positive and CP maps introduced in Sec. 1.1.1 have a bijective correspondence between positive and CP maps of C*-algebras.

On the other hand, when C*-algebras are commutative, positive (=CP) maps of C*-algebras have bijective correspondence between transition matrices. If X_A and X_B are finite sets representing random variables, the sets of continuous functions $\mathrm{Cont}(X_A, \mathbb{C})$ and $\mathrm{Cont}(X_B, \mathbb{C})$ from X_A and X_B form commutative C*-algebras. The multiplication and summation are defined by that of functions. Then there is a bijective correspondence between transition matrices from X_B to X_A and unital positive (=CP) maps of C*-algebras from $\mathrm{Cont}(X_A, \mathbb{C})$ to $\mathrm{Cont}(X_B, \mathbb{C})$ (see, e.g. Ref. [60]). If $[f(x_B)(x_A)]_{x_B \in X_B,\ x_A \in X_A}$ is a transition matrix from X_B to X_A, it induces a positive (=CP) map f_* by

$$f_* : g \mapsto \sum_{x_A \in X_A} f(\cdot)(x_A) g(x_A) \qquad (\forall g : X_A \to \mathbb{C}). \tag{1.22}$$

In the right of this bijective correspondence $f \leftrightarrow f_*$, we regard transition matrices as positive (=CP) maps in classical probability theory.

1.3.3 Classical Markov chains

A sequence of random variables $X_1,\ X_2, ...,\ X_n$ is called a stochastic process under the assumption that these random variables obey a joint probability distribution $p : X_1 \times X_2 \times ... \times X_n \to [0, 1]$. Markov chains are usually defined as a particular kind of stochastic processes [50]. In this thesis, however, we define Markov chains as a particular kind of joint probability distributions, rather not of stochastic processes.

A joint distribution p on $X_1,\ X_2, ...,\ X_n$ is called a Markov chain if

$$p_{X_i|X_{i-1}\times\ldots\times X_1}(x_i|x_{i-1}, .., x_1) = p_{X_i|X_{i-1}}(x_i|x_{i-1})$$

holds for all i and $x_j \in X_j$ $(j = 1, ..., i)$. This condition states that the probability for random variable X_i depends on $X_{i-2},\ X_{i-3}, ...,\ X_1$ only through X_{i-1}.

Equivalently, random variables $X_1,\ X_2, ...,\ X_n$ constitute of a Markov chain if the joint distribution decomposes to

$$p_{X_n\ldots X_1}(x_n, ..., x_1) = f_{X_n|X_{n-1}}(x_{n-1})(x_n)\ldots f_{X_2|X_1}(x_1)(x_2)p_{X_1}(x_1), \tag{1.23}$$

where p_{X_1} is a probability distribution on X_1, and $f_{X_i|X_{i-1}}$ are transition matrices from X_{i-1} to X_i.

Expression (1.23) of Markov chains reveals a method to extend Markov chains to arbitrary lengths by transition matrices. We generalise this expression by using Kleisli categories of monads in Chap. 6. We give an introduction to monads in Sec. 1.3.4, and to a particular monad to express probability distributions in Sec. 1.3.5. After these introductions, we reformulate the Expr. (1.23) of classical Markov chains category theoretically in Sec. 1.3.3.

1.3.4 Monad and Kleisli category

We recall definitions of monad and its Kleisli category to represent probability distributions and transition matrices categorically in the next subsection. Familiarity of basic category theory presented in Appx. C.1 and Appx. C.2 is required.

When we use category theory, $\mathrm{id}_{\mathbf{C}}$ represents the identity functor on category $\mathbf{C}$. There would be no confusion with the identity map $\mathrm{id}_{\mathcal{H}}$ on operator spaces $\mathcal{B}(\mathcal{H})$.

Definition 3 (monad)**.** Let $\mathbf{C}$ be a category. A triple (T, η, μ) of functor $T : \mathbf{C} \to \mathbf{C}$, natural transformations $\eta : \mathrm{id}_{\mathbf{C}} \to T$ and $\mu : T^2 \to T$ is called monad, if they make following diagrams commute for any object X of $\mathbf{C}$:

$$\begin{array}{ccc} T^3X & \xrightarrow{T\mu_X} & T^2X \\ \downarrow{\scriptstyle \mu_{TX}} & & \downarrow{\scriptstyle \mu_X} \\ T^2X & \xrightarrow{\mu_X} & TX, \end{array} \qquad \begin{array}{ccc} TX & \xrightarrow{T\eta_X} & T^2X \\ {\scriptstyle \eta_{TX}}\downarrow & \overset{\cong}{=\!=} & \downarrow{\scriptstyle \mu_X} \\ T^2X & \xrightarrow[\mu_X]{} & TX. \end{array} \tag{1.24}$$

The natural transformation η and μ are called unit and multiplication of the monad (T, η, μ). An example will be given in Sec. 1.3.5 by the distribution monad.

The Kleisli category of a monad is defined as follows. Objects of the Kleisli category of monad (T, η, μ) on $\mathbf{C}$ are objects of $\mathbf{C}$. Morphisms of the Kleisli category from object X to object Y are morphisms $X \to TY$ in $\mathbf{C}$. We call the morphisms in Kleisli category by Kleisli morphisms and denote them by arrows $\to_{\mathcal{K}\ell}$, so that $f : X \to_{\mathcal{K}\ell} Y$ represents $f : X \to TY$ in $\mathbf{C}$. The identity morphisms in the Kleisli category are unit morphisms ν_X. The composition of Kleisli morphisms, Kleisli composition for short, of $f : X \to_{\mathcal{K}\ell} Y$ and $g : Y \to_k lZ$ is defined by the composition

$$\mu_Z \circ (Tg) \circ f \tag{1.25}$$

in $\mathbf{C}$, and is denoted by $g \odot f : X \to_{\mathcal{K}\ell} Z$.

Classical probability theory has a notion of product distributions on composite random variables. To generalise the notion of product distributions, monads are requred to be strong, defined as below.

Definition 4. [61, Def. 3.2] A monad (T, η, μ) on symmetric monoidal category $(\mathbf{C}, \otimes, I)$ is said to be *strong*, if there is a set of morphisms

$$\mathrm{st}_{X,Y} : X \otimes TY \to T(X \otimes Y), \tag{1.26}$$

natural in both arguments X and Y, such that

$$\begin{array}{ccc} TX & & \\ \uparrow{\scriptstyle r_X} & \nwarrow{\scriptstyle Tr_X} & \\ I \otimes TX & \xrightarrow[\mathrm{st}_{I,X}]{} & T(I \otimes X), \end{array} \tag{1.27}$$

$$\begin{array}{ccccc} (X \otimes Y) \otimes TZ & \xrightarrow{\mathrm{st}_{X\otimes Y,Z}} & T((X \otimes Y) \otimes Z) & & \\ \downarrow{\scriptstyle \alpha_{X,Y,TZ}} & & & \searrow{\scriptstyle T\alpha_{X,Y,Z}} & \\ X \otimes (Y \otimes TZ) & \xrightarrow[\mathrm{id}_X \otimes \mathrm{st}_{Y,Z}]{} & X \otimes T(Y \otimes Z) & \xrightarrow[\mathrm{st}_{X \otimes (Y \otimes Z)}]{} & T(X \otimes (Y \otimes Z)), \end{array} \tag{1.28}$$

$$\begin{array}{ccccc} X \otimes Y & & & & \\ \downarrow{\scriptstyle \mathrm{id}_X \otimes \eta_Y} & \searrow{\scriptstyle \eta_{X\otimes Y}} & & & \\ X \otimes TY & \xrightarrow[\mathrm{st}_{X,Y}]{} & T(X \otimes Y) & & \\ \uparrow{\scriptstyle \mathrm{id}_X \otimes \mu_Y} & & & \nwarrow{\scriptstyle \mu_{X\otimes Y}} & \\ X \otimes T^2Y & \xrightarrow[\mathrm{st}_{X,TY}]{} & T(X \otimes TY) & \xrightarrow[T\mathrm{st}_{X,Y}]{} & T^2(X \otimes Y), \end{array} \tag{1.29}$$

where r and α are natural isomorphisms of

$$r_X : I \otimes X \to X, \qquad \alpha_{X,Y,Z} : (X \otimes Y) \otimes Z \to X \otimes (Y \otimes Z). \tag{1.30}$$

The natural transformation st is called the *strength*. Conjugating with the swap morphism c induces a natural transformation

$$\mathrm{cst}_{X,Y} = c \circ \mathrm{st}_{Y,X} \circ c : TX \otimes Y \to T(X \otimes Y), \tag{1.31}$$

called the *costrength*. Two morphisms called *Fubini maps* are constructed by

$$\mathrm{dst}_{X,Y} \ : \ TX \otimes TY \xrightarrow{\mathrm{cst}_{X,TY}} T(X \otimes TY) \xrightarrow{T\mathrm{st}_{X,Y}} T^2(X \otimes Y) \xrightarrow{\mu_{X\otimes Y}} T(X \otimes Y), \tag{1.32}$$

$$\mathrm{dst}'_{X,Y} \ : \ TX \otimes TY \xrightarrow{\mathrm{st}_{TX,Y}} T(TX \otimes Y) \xrightarrow{T\mathrm{cst}_{X,Y}} T^2(X \otimes Y) \xrightarrow{\mu_{X\otimes Y}} T(X \otimes Y). \tag{1.33}$$

Fubini maps are known to be natural transformations (natural with regard to both arguments X and Y). These two Fubini maps do not necessarily coincide, but if they do, the strong monad is said to be *commutative.*

The Fubini map for the distribution monad is unique since it is commutative. As we will see in Sec. 1.3.5, it plays a role to make product distributions from two marginal distributions.

1.3.5 Distribution monad

Here we review the distribution monad, and reformulate classical Markov chains categorically in the next subsection. Our goal is to express the process to extend Markov chains as Expr. (1.23) by a composition of Kleisli morphisms of the distribution monad (cf. Eq. (1.45)).

The distribution monad $(\mathscr{D},\ \eta,\ \mu)$ is a monad over **Sets**, and thus all the morphisms are functions. Its functor part $\mathscr{D}\colon \mathbf{Sets} \to \mathbf{Sets}$ is defined by (see Ref. [62, 63]):

$$\mathscr{D}(A) = \{p\colon A \to [0,1] \mid \mathrm{supp}(p) \text{ finite}, \sum_{a\in A} p(a) = 1\},$$
$$\mathscr{D}(f)(r_1\delta_1 + r_2\delta_2 + \dots + r_n\delta_n) = r_1\delta_{f(1)} + r_2\delta_{f(2)} + \dots + r_n\delta_{f(n)},$$

for set A and function f, where δ denotes Kronecker's delta function and $\sum_{i=1}^{n} r_i = 1$ with $r_i \in [0,1]$. Its unit and multiplication are defined by

$$\eta_A\colon A \to \mathscr{D}(A) \qquad\qquad \mu_A\colon \mathscr{D}^2(A) \to \mathscr{D}(A)$$
$$a \mapsto \delta_a \qquad\qquad r_1\delta_{p_1} + r_2\delta_{p_2} + \dots + r_n\delta_{p_n} \mapsto r_1p_1 + r_2p_2 + \dots + r_np_n.$$

The distribution monad is strong and commutative. Although we do not show the strength and costrength, the unique Fubini map $i_{X,Y} : \mathscr{D}X \times \mathscr{D}Y \to \mathscr{D}(X \times Y)$ represents the inclusion of marginal distributions to form a product distribution on $X \times Y$:

$$i : (p_X, p_Y) \mapsto p_X \times p_Y. \tag{1.34}$$

The Kleisli category of the distribution monad is the category of probability distributions [64]. A Kleisli morphism $f : X \to_{\mathcal{K}\ell} Y$ maps points of X to probability distributions on Y, and usually expressed by a $|X|$-by-$|Y|$ transition matrix $[f(x)(y)]_{x\in X,\ y\in Y}$ with entries $f(x)(y) \in [0,1]$ satisfying $\sum_y f(x)(y) = 1$ for all $x \in X$. This expression of a transition matrix is meant to represent that a point $x \in X$ is mapped to a probability distribution $f(x) : Y \to [0,1]$ on Y. In particular, Kleisli morphisms $1 \to_{\mathcal{K}\ell} X$ with 1 as the terminal object $1 = \{*\}$ (singleton set) are probability distributions on X. Kleisli categories of monads have been widely used to express stochastic processes since Giry has discovered a monad for probability measures [63].

The Kleisli composition of transition matrices comes down to matrix multiplication. If $f : W \to_{\mathcal{K}\ell} X$ and $g : X \to_{\mathcal{K}\ell} Y$ are expressed by transition matrices $[f(w)(x)]_{w\in W,\ x\in X}$ and $[g(x)(y)]_{x\in X,\ y\in Y}$, respectively, the transition matrix for

$g \odot f = (\mu_Y \circ \mathscr{D}(g) \circ f)$ is

$$\begin{aligned}(\mu_Y \circ \mathscr{D}(g) \circ f)(w)(y) &= (\mu_Y \circ \mathscr{D}(g)) \left(\sum_{x \in X} f(w)(x) \delta_x \right) (y) && (1.35) \\ &= \mu_Y \left(\sum_{x \in X} f(w)(x) \delta_{g(x)} \right) (y) && (1.36) \\ &= \left(\sum_{x \in X} f(w)(x) g(x) \right) (y) && (1.37) \\ &= \sum_{x \in X} f(w)(x) g(x)(y). && (1.38)\end{aligned}$$

If W is the terminal object $1 = \{*\}$, then the composition $g \odot f$ is a probability distribution

$$\sum_{x \in X} f(*)(x) g(x)(y) = \sum_{x \in X} p(x) g(x)(y), \tag{1.39}$$

on Y, where $[p(x)]_{x \in X}$ is the probability distribution on X defined by $p(x) = f(*)(x)$.

1.3.6 Representing Markov chains by Kleisli compositions

There is sill the difference between multiplication of transition matrices presented in Eq. (1.23) for Markov chains and Eq. (1.39) for the Kleisli composition. The summation on the middle variable (X in Eq. (1.39)) is not taken for Markov chains.

The summation on the middle variable can be avoided in the following way. Let $p : 1 \to_{\mathcal{K}\ell} X$ and $g : X \to_{\mathcal{K}\ell} Y$ be Kleisli morphisms corresponding to probability distribution $[p(x)]_{x \in X}$ and transition matrix $[g(x)(y)]_{x \in X,\ y \in Y}$. We consider the Kleisli composition of p and

$$i \circ \langle g, \eta_X \rangle : X \to_{\mathcal{K}\ell} X \times Y, \tag{1.40}$$

where $i : \mathscr{D}X \times \mathscr{D}Y \to \mathscr{D}(X \times Y)$ is the Fubini map. Morphism $g : X \to_{\mathcal{K}\ell} Y$ is coupled with $\eta_X : X \to_{\mathcal{K}\ell} X$ to form a morphism from a single system to a joint system. The Kleisli composition

$$(i \circ \langle g, \eta_X \rangle) \odot p : 1 \to_{\mathcal{K}\ell} X \times Y, \tag{1.41}$$

corresponds to a joint distribution

$$\begin{aligned} & (\mu_{X \times Y} \circ \mathscr{D}(i \circ \langle g, \eta_X \rangle) \circ p)(*)(x, y) \\ = & \left((\mu_{X \times Y} \circ \mathscr{D}(i \circ \langle g, \eta_X \rangle)) \left(\sum_{x' \in X} p(x') \delta_{x'} \right) \right) (x, y) \\ = & \mu_{X \times Y} \left(\sum_{x' \in X} p(x') \delta_{g(x') \times \delta_{x'}} \right) (x, y) \\ = & \left(\sum_{x' \in X} p(x') g(x') \times \delta_{x'} \right) (x, y) \\ = & p(x) g(x)(y). && (1.42)\end{aligned}$$

on $X \times Y$. We do not have the summation over X in Eq. (1.42).

We have extended a single probability distribution to a bipartite one by using the Kleisli morphism presented in Eq. (1.40). For defining Markov chains, we have to extend bipartite Markov chains into tripartite ones. This can be easily done by a slight reformulation of Def. (1.40). To extend the bipartite Markov chain presented in Eq. (1.42) to

$$p(x)g(x)(y)h(y)(z), \tag{1.43}$$

by a transition matrix $[h(y)(z)]_{y\in Y,\ z\in Z}$, simply compose

$$\mathrm{ext} := i_{X,Y\times Z} \circ (\eta_X \times i_{Y,Z} \circ \langle \eta_Y, h\rangle) : X \times Y \to_{\mathcal{K}\ell} X \times Y \times Z \tag{1.44}$$

and the joint distribution presented by Def. (1.41). The unit morphism η_X on X preserves the marginal X, and $i_{Y,Z} \circ \langle \eta_Y, h\rangle$ extends Y to $Y \times Z$ via transition matrix h to produce

$$\mathrm{ext} \odot (i \circ \langle g, \eta_X\rangle) \odot p : 1 \to_{\mathcal{K}\ell} X \times Y \times Z, \tag{1.45}$$

which is equivalent to the tripartite Markov chain (1.43).

We have expressed the Markov chain presented in Eq. (1.23) in terms of the Kleisli composition of the distribution monad. It is now clear how to extend Markov chains to longer ones by transition matrices. In Chap. 6, we define Markov chains for other strong monads by a direct generalisation of Eq. (1.45), and investigate their properties with a special attention to topos quantum theory.

Chapter 2

Positive non-CP maps and supermaps

We have already reviewed the defining properties of positive non-CP maps in the previous chapter. The positive non-CP maps and supermaps are sound if they are performed on single systems, but not on parts of composite systems (see Sec. 1.1.1). They are not straightforwardly realisable by quantum manipulators since they are not CP (see Sec. 1.1.2). In this chapter, we review more detailed properties of the positive non-CP maps and supermaps used in this thesis.

In Sec. 2.1, we focus on positive non-CP *maps*, and summarise their properties used in Chaps. 3 and 5. In Sec. 4, we turn to positive non-CP *supermaps*. We introduce the positive non-CP supermap, namely channel transposition, investigated in Chap. 4, and review a related preceding work. Finally in Sec. 2.3, we give an introduction to quantities defined by using conjugation operators. Our analysis in Chaps. 3 and 4 provides a method to compute these quantities.

2.1 Positive non-CP maps

As we have mentioned in the introduction, positive and CP maps differ in quantum theory, while they are equivalent in classical probability theory. We review the gap between positive and CP maps and its relation to positive over pure tensor states in Sec. 2.1.1. These states appear in our definition of composite systems in topos quantum theory presented in Chap. 5. Section 2.1.2 reviews a preceding work Ref. [27] on an approximation of a positive non-CP map, based on which we prove a no-go theorem for state transposition in Chap. 3.

2.1.1 Representation of positive maps

The Choi isomorphism provides a bijective correspondence between positive maps to 1-positive operators. We give a detailed introduction to 1-positive operators and its multipartite generalisation.

A bipartite operator $\omega \in \mathcal{B}(\mathcal{H} \otimes \mathcal{K})$ is said to be 1-positive if

$$\mathrm{Tr}[\omega |\psi\rangle\langle\psi| \otimes |\phi\rangle\langle\phi|] \geq 0 \tag{2.1}$$

for any pair of quantum states $|\psi\rangle$ on $\mathcal{H}$ and $|\phi\rangle$ on $\mathcal{K}$. This definition implies that 1-positive operators are positive over all product positive semi-definite operators:

$$\mathrm{Tr}[\omega P_{\mathcal{H}} \otimes P_{\mathcal{K}}] \geq 0 \qquad (\forall P_{\mathcal{H}} \in \mathrm{Pos}(\mathcal{H}),\ \forall P_{\mathcal{K}} \in \mathrm{Pos}(\mathcal{K})). \tag{2.2}$$

Let us consider the Choi operator for transposition $\mathrm{T} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ as an example. For simplicity, we take the basis for operator $\Phi_{\mathcal{H},\mathcal{H}} := \sum_{i,j=1}^{\dim \mathcal{H}} |i,i\rangle\langle j,j|$ so that the transposition is taken in the same basis. The Choi operator of transposition is

$$\widetilde{\mathrm{T}} := \mathrm{id}_{\mathcal{H}} \otimes \mathrm{T}(\sum_{i,j=1}^{\dim \mathcal{H}} |i,i\rangle\langle j,j|) = \sum_{i,j=1}^{\dim \mathcal{H}} |i,j\rangle\langle j,i| =: \mathrm{SWAP}_{\mathcal{H}\otimes\mathcal{H}}, \tag{2.3}$$

where $\mathrm{SWAP}_{\mathcal{H}\otimes\mathcal{H}}$ represents the swap operator that exchanges vectors on two Hilbert spaces $\mathcal{H}$. The swap operator is not positive semi-definite. It has eigenvectors with negative eigenvalues.

The 1-positive operators that are not positive are called entanglement witnesses. They are used as observables for detecting entanglement. See [11] for example for a review of entanglement witness.

Unit trace 1-positive operators are called positive over pure tensor states [65]. They are similar to quantum states, and the gap between positive over pure tensor states and quantum states corresponds to the gap between positive maps and CP maps. To see this correspondence, let us consider a bipartite quantum state $\rho \in \mathcal{S}(\mathcal{H}_1 \otimes \mathcal{K})$ and a positive TP map $\mathcal{F} : \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{H}_2)$. The operator

$$\mathcal{F} \otimes \mathrm{id}_{\mathcal{K}}(\rho) \tag{2.4}$$

is not necessarily positive if $\mathcal{F}$ is not CP. It is, however, always a positive over pure tensor state because

$$\begin{aligned}\mathrm{Tr}[\mathcal{F} \otimes \mathrm{id}_{\mathcal{K}}(\rho)|\psi\rangle\langle\psi| \otimes |\phi\rangle\langle\phi|] &= \mathrm{Tr}[\rho\mathcal{F}^{\dagger}(|\psi\rangle\langle\psi|) \otimes |\phi\rangle\langle\phi|] \geq 0, \\ &\quad (\forall|\psi\rangle\langle\psi| \in \mathcal{S}(\mathcal{H}_2),\ \forall|\phi\rangle\langle\phi| \in \mathcal{S}(\mathcal{K}))\end{aligned}$$

where $\mathcal{F}^{\dagger} : \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_1)$ is the dual map for $\mathcal{F}$ (see Appx. A for the definition). Conversely, all the positive over pure tensor states that are not quantum states are generated by the action of positive TP maps applied on a part of quantum multipartite quantum states [65].

Actions of positive non-CP maps applied on a part of multi-party quantum system are never physically realisable since they transform entangled quantum states to positive over pure tensor states that are not necessarily valid quantum states. We assume that the input states and maps are uncorrelated to other systems when considering realisability of positive non-CP maps and supermaps in Chaps. 3 and 4. The unrealisablity of positive non-CP maps and supermaps on the uncorrelated states and maps does not straightforwardly follow from the unrealisability of the actions on marginal systems.

The definition of positive over pure tensor states can be generalised to multipartite systems.

Definition 5 (positive over pure tensor states)**.** Let $\mathcal{H}_i$ $(i = 1, ..., n)$ be Hilbert spaces. A bounded linear operator ω on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ is said to be a positive over pure tensor state if $\mathrm{Tr}[\omega] = 1$ and

$$\mathrm{Tr}[(P_1 \otimes ... \otimes P_N)\omega] \geq 0,$$

is satisfied for any set of positive operators P_i on $\mathcal{H}_i$.

The set of all positive over pure tensor states on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ is denoted by $\mathcal{W}(\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n)$. The state space $\mathcal{W}(\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n)$ is convex in the sense probabilistic mixture of any positive over pure tensor states is again a positive over pure tensor state. For the bipartite case, the extremal points of $\mathcal{W}(\mathcal{H} \otimes \mathcal{K})$ are characterised in Ref. [66], and pure quantum states and their partial transpositions are the examples of extremal bipartite positive over pure tensor states. We deduce several properties of positive over pure tensor states from this fact which will be applied to the topos quantum theory in Chap. 6.

2.1.2 Approximation of non-CP map

Quantum manipulators cannot perform positive non-CP maps deterministically, since they are not CP. If one knows the description of the input state, however, any map is realisable by calculating the description of the output state and generating it. If infinite clones of the unknown state are given, one may perform state tomography and obtain the description of the state. Thus giving infinite clones of the unknown state is sufficient to realise any map on the state.

If finite clones of the unknown state are given, it is possible to approximate the non-CP map. The approximation will be increasingly improved when more clones are given. Here, we review a preceding work on approximation of a non-CP map called the "universal-NOT" transformation [27]. We use this result to derive the necessity of infinite clones for probabilistic state transposition in Sec. 3.1.

For any pure state $|\psi\rangle \in \mathbb{C}_2$ in a two dimensional Hilbert space, there is a (up to phase) unique state $|\psi^\perp\rangle$ that is orthogonal to $|\psi\rangle$, namely, satisfying $\langle\psi|\psi^\perp\rangle = 0$. A mapping

$$|\psi\rangle\langle\psi| \mapsto |\psi^\perp\rangle\langle\psi^\perp| \qquad (\forall|\psi\rangle \in \mathbb{C}_2), \tag{2.5}$$

is named the universal-NOT transformation because its classical analogue is the NOT-gate on a bit whose action is represented by $0 \mapsto 1$ and $1 \mapsto 0$. A linear map $\mathcal{B}(\mathbb{C}_2) \to \mathcal{B}(\mathbb{C}_2)$ satisfying Eq. (2.5) for all pure states is positive and TP, but inevitably non-CP. The linear map is decomposed into

$$\mathcal{U}[\sigma_y] \circ \mathrm{T}, \tag{2.6}$$

and the non-CP nature is provided by T. The other expression of the universal-NOT which was chosen in Ref. [27] is $\mathcal{U}[\sigma_y\Theta]$ with a conjugation operator Θ (see Sec. 2.3.1 for an equivalence of conjugation and transposition).

It is impossible to deterministically implement the universal-NOT transformation on an unknown pure state $|\psi\rangle$ since it is not expressed by a TPCP map. Then it is natural to ask the optimal approximation of for the universal-NOT transformation. In Ref. [27], the authors consider the optimal approximation of universal-NOT transformation under the assumption that finite clones of the unknown state $|\psi\rangle$ are given. They seek for a TPCP map $\Gamma : \mathcal{B}(\mathbb{C}_2^{\otimes n}) \to \mathcal{B}(\mathbb{C}_2)$ such that $\Gamma(|\psi\rangle\langle\psi|^{\otimes n})$ approximates state $|\psi^\perp\rangle\langle\psi^\perp|$. The figure of merit they use for measuring the accuracy of the approximation is the worst case fidelity

$$\mathrm{F}_n(\Gamma) := \min_{|\psi\rangle} \mathrm{Tr}\left[|\psi^\perp\rangle\langle\psi^\perp|\Gamma(|\psi\rangle\langle\psi|^{\otimes n})\right], \tag{2.7}$$

where the minimum is taken over all pure states in $\mathbb{C}_2$. This fidelity becomes 1 if Γ perfectly implements the universal-NOT, i.e. if $\Gamma(|\psi\rangle\langle\psi|^{\otimes n}) = |\psi^\perp\rangle\langle\psi^\perp|$ for all $|\psi\rangle$, and approaches to 1 as $\Gamma(|\psi\rangle\langle\psi|^{\otimes n})$ becomes indistinguishable from $|\psi^\perp\rangle\langle\psi^\perp|$. They derive the following optimal fidelity for the universal-NOT transformation:

$$\max_{\Gamma:\mathcal{B}(\mathbb{C}_2^{\otimes n})\to\mathcal{B}(\mathbb{C}_2),\ \text{TPCP map}} \mathrm{F}_n(\Gamma) = 1 - \frac{1}{n+2}. \tag{2.8}$$

The scaling of this optimal fidelity with respect to n is important for our impossibility proof presented in Sec. 3.1.

2.2 Positive non-CP supermap

In the previous section, we reviewed the gap between positive and CP maps, and also reviewed a related preceding work. Here we turn to the supermaps. As we have mentioned in the introduction and Sec. 1.2.2, there also exists a gap between positive and CP supermaps. We show an example of positive non-CP supermap, channel transposition, in Sec. 2.2.1. The channel transposition becomes our main concern in Chap. 4. Although not directly used in our work, we review a preceding work on channel transposition in Sec. 2.2.2, to clarify the novelty of our work presented in Chap 4.

2.2.1 Channel transposition

Let $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ be a CP map, $\mathrm{T}_\mathcal{H}$ and $\mathrm{T}_\mathcal{K}$ be transpositions on $\mathcal{H}$ and $\mathcal{K}$, respectively. Positive maps defined by $\mathrm{T}_\mathcal{K} \circ \mathcal{E}$ and $\mathcal{E} \circ \mathrm{T}_\mathcal{H}$ are not necessarily CP since transpositions are not. The CP map sandwiched by transpositions, i.e.

$$\mathrm{T}_\mathcal{K} \circ \mathcal{E} \circ \mathrm{T}_\mathcal{H}, \tag{2.9}$$

is, however, again CP. Here, we show that the supermap $\mathcal{E} \mapsto \mathrm{T}_\mathcal{K} \circ \mathcal{E} \circ \mathrm{T}_\mathcal{H}$ is positive but not CP, and introduce an useful representation for the supermap.

Let $\widetilde{\mathcal{E}} \in \mathrm{Pos}(\mathcal{H} \otimes \mathcal{K})$ be the Choi operator of $\mathcal{E}$ defined by Eq. (1.15). We take the defining basis of the operator $\Phi_{\mathcal{H},\mathcal{H}} := (\sum_{i=1}^{\dim\mathcal{H}} |i,i\rangle)(\sum_{i=1}^{\dim\mathcal{H}} \langle i,i|)$ so that transposition $\mathrm{T}_\mathcal{H}$ is taken in the same basis. In this basis, we can swap the Hilbert space taken partial transposition as

$$\mathrm{T}_\mathcal{H} \otimes \mathrm{id}_\mathcal{H}(\Phi_{\mathcal{H},\mathcal{H}}) = \sum_{i,j=1}^{\dim\mathcal{H}} |j,i\rangle\langle i,j| = \mathrm{id}_\mathcal{H} \otimes \mathrm{T}_\mathcal{H}(\Phi_{\mathcal{H},\mathcal{H}}). \tag{2.10}$$

Since transpositions are positive map and their spatial composition $\mathrm{T}_{\mathcal{H}} \otimes \mathrm{T}_{\mathcal{K}} = \mathrm{T}_{\mathcal{H}\otimes\mathcal{K}}$ is again transposition,

$$\begin{aligned} \mathrm{T}_{\mathcal{H}\otimes\mathcal{K}}\widetilde{\mathcal{E}} &= \mathrm{T}_{\mathcal{H}} \otimes (\mathrm{T}_{\mathcal{K}} \circ \mathcal{E})(\Phi_{\mathcal{H},\mathcal{H}}) = \mathrm{id}_{\mathcal{H}} \otimes (\mathrm{T}_{\mathcal{K}} \circ \mathcal{E} \circ \mathrm{T}_{\mathcal{H}})(\Phi_{\mathcal{H},\mathcal{H}}) \quad (2.11) \\ &= \widetilde{(\mathrm{T}_{\mathcal{K}} \circ \mathcal{E} \circ \mathrm{T}_{\mathcal{H}})} \quad (2.12) \end{aligned}$$

is positive semi-definite. Here we swapped the Hilbert space taken partial transposition $\mathrm{T}_{\mathcal{H}}$ in the second equality. Since the Choi isomorphism provides a bijective correspondence between CP maps and positive semi-definite operators, $\mathrm{T}_{\mathcal{K}} \circ \mathcal{E} \circ \mathrm{T}_{\mathcal{H}}$ is CP.

When $\mathcal{E}$ is TP, $\mathrm{T}_{\mathcal{K}} \circ \mathcal{E} \circ \mathrm{T}_{\mathcal{H}}$ is again TP since the transposition preserves trace. We call the mapping from TPCP map $\mathcal{E}$ to TPCP map $\mathrm{T}_{\mathcal{K}} \circ \mathcal{E} \circ \mathrm{T}_{\mathcal{H}}$ the *channel transposition*. The Choi isomorphism reduces the channel transposition to usual transposition on Choi operators, and thus the channel transposition is an example of a positive non-CP supermap defined in Sec. 1.2.2. We investigate the physical realisability of the channel transposition in Chap. 4.

A representation of CP maps called "Kraus decomposition" simplifies the description of the channel transposition. A linear map $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ is CP if and only if there is a set of operators $\{E_i\}$ all in $\mathcal{B}(\mathcal{H}, \mathcal{K})$, such that

$$\mathcal{E} = \sum_i \mathcal{U}[E_i]. \quad (2.13)$$

The map $\mathcal{E}$ is further TP (TNI) if $\sum_i E_i^\dagger E_i = \mathbb{I}_{\mathcal{H}}$ ($\sum_i E_i^\dagger E_i \leq \mathbb{I}_{\mathcal{H}}$). The operators E_i are called Kraus operators for $\mathcal{E}$, and the representation of CP map presented in Eq. (2.13) is called the Kraus decomposition of $\mathcal{E}$. Trivial examples are given by unitary channels $\mathcal{U}[U]$, where in this case there is only one Kraus operator U.[1]

Let $\mathcal{E} = \sum_i \mathcal{U}[E_i]$ be a Kraus decomposition of TPCP map $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$, and O be an operator on $\mathcal{H}$. The action of transposed channel $\mathrm{T}_{\mathcal{K}} \circ \mathcal{E} \circ \mathrm{T}_{\mathcal{H}}$ on O reduces to

$$\begin{aligned} \mathrm{T}_{\mathcal{K}} \circ \mathcal{E} \circ \mathrm{T}_{\mathcal{H}}(O) &= \sum_i \left(E_i O^{\mathrm{T}} E_i^\dagger\right)^{\mathrm{T}} = \sum_i (E_i^\dagger)^{\mathrm{T}} (O^{\mathrm{T}})^{\mathrm{T}} (E_i)^{\mathrm{T}} \quad (2.14) \\ &= \sum_i E_i^* O (E_i^*)^\dagger, \quad (2.15) \end{aligned}$$

where the transpositions and complex conjugations are taken in the basis of $\mathrm{T}_{\mathcal{K}}$ and $\mathrm{T}_{\mathcal{H}}$. Since this holds for any operator O on $\mathcal{H}$, a Kraus decomposition of the transposed TPCP map $\mathrm{T}_{\mathcal{K}} \circ \mathcal{E} \circ \mathrm{T}_{\mathcal{H}}$ is provided by the conjugated Kraus operators E_i^*.

[1] By using the Kraus decomposition of TNICP map $\mathcal{E}$, we can construct the TNICP map $\mathcal{E}'$ such that $\{\mathcal{E}, \mathcal{E}'\}$ becomes an instrument, as described in Sec. 1.1.2. If $\mathcal{E} = \sum_i \mathcal{U}[E_i]$ is a Kraus decomposition of $\mathcal{E}$, the operator $\mathbb{I}_{\mathcal{H}} - \sum_i E_i^\dagger E_i$ is positive semi-definite since $\mathcal{E}$ is TNI. It is possible to construct the operator E' such that $E'^\dagger E' = \mathbb{I}_{\mathcal{H}} - \sum_i E_i^\dagger E_i$. Define $\mathcal{E}'$ by its Kraus decomposition $\mathcal{E}' := \mathcal{U}[E']$. Then $\mathcal{E} + \mathcal{E}'$ has Kraus decomposition $\mathcal{U}[E'] + \sum_i \mathcal{U}[E_i]$ and is TP because $E'^\dagger E' + \sum_i E_i^\dagger E_i = \mathbb{I}_{\mathcal{H}}$. Since quantum manipulators can perform any instruments, and since any TNICP maps are extendible to instruments in this way, any TNICP maps are probabilistically realisable by quantum manipulators.

In particular for unitary channels, the channel transposition outputs the conjugated unitary channel

$$\mathrm{T} \circ \mathcal{U}[U] \circ \mathrm{T} = \mathcal{U}[U^*]. \tag{2.16}$$

We call the mapping $\mathcal{U}[U] \mapsto \mathcal{U}[U^*]$ by *unitary conjugation*, to avoid a potential confusion with the transposition on unitary operators $U \mapsto U^{\mathrm{T}}$. We investigate the realisability of the unitary conjugation in Chap. 4.

2.2.2 Approximation of positive non-CP supermap

Although we will be interested in probabilistic exact realisations of the unitary conjugation in Chap. 4, it is also possible to approximate realisations. An approximation of the unitary conjugation without replication is investigated in Ref. [29]. We do not apply their technique to our work, but review their results to delineate the difference between preceding works and ours.

Let $U : \mathcal{H} \to \mathcal{K}$ be a unitary operator on $\mathcal{H} \cong \mathcal{K}$, where the dimension of Hilbert spaces is denoted by d. We consider implementing an approximation of $\mathcal{U}[U^*]$ from a given unknown unitary channel $\mathcal{U}[U]$. Since the replicas of $\mathcal{U}[U]$ are not given, a deterministically realisable supermap is characterised by the pair of TPCP maps, encoder $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H} \otimes \mathcal{H}_A)$ and decoder $\mathcal{B}(\mathcal{K} \otimes \mathcal{H}_A) \to \mathcal{B}(\mathcal{K})$, with which a TPCP map

$$\Gamma_U^{\mathcal{E},\mathcal{D}} := \mathcal{D} \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \mathcal{U}[U]) \circ \mathcal{E}, \tag{2.17}$$

is implemented (cf. Eq. (1.12)). In Ref. [29], authors used the channel fidelity as the figure of merit measuring the accuracy of approximation. It is defined as the fidelity between normalised Choi matrices of the target TPCP map and the approximating TPCP map. For the unitary conjugation,

$$\mathrm{F}(\mathcal{U}[U^*], \Gamma_U^{\mathcal{E},\mathcal{D}}) := \frac{1}{d^2} \mathrm{Tr}\left[(\mathbb{I}_{\mathcal{H}} \otimes \mathcal{U}[U^*])(\Phi_{\mathcal{H},\mathcal{H}})(\mathbb{I}_{\mathcal{H}} \otimes \Gamma_U^{\mathcal{E},\mathcal{D}})(\Phi_{\mathcal{H},\mathcal{H}}) \right], \tag{2.18}$$

where $\Phi_{\mathcal{H},\mathcal{H}}$ is a density operator of maximally entangled state $\sum_{i=1}^{d} |i, i\rangle$. The fidelity $\mathrm{F}(\mathcal{U}[U^*], \Gamma_U^{\mathcal{E},\mathcal{D}})$ becomes 1 if $\Gamma_U^{\mathcal{E},\mathcal{D}}$ coincides with $\mathcal{U}[U]$, and decreases as the approximation becomes worse.[2]

They have shown that the maximum of the averaged fidelity

$$\int dU \; \mathrm{F}(\mathcal{U}[U^*], \Gamma_U^{\mathcal{E},\mathcal{D}}), \tag{2.21}$$

[2]As another figure of merit, one may consider

$$f_{|\psi\rangle}(\mathcal{U}[U^*], \Gamma_U^{\mathcal{E},\mathcal{D}}) := \mathrm{Tr}[\mathcal{U}[U^*](|\psi\rangle\langle\psi|)\Gamma_U^{\mathcal{E},\mathcal{D}}(|\psi\rangle\langle\psi|)]. \tag{2.19}$$

The fidelity $\mathrm{F}(\mathcal{U}[U^*], \Gamma_U^{\mathcal{E},\mathcal{D}})$ is related to $f_{|\psi\rangle}(\mathcal{U}[U^*], \Gamma_U^{\mathcal{E},\mathcal{D}})$ by

$$\int dU' f_{U'|\psi\rangle} = \frac{\mathrm{F}(\mathcal{U}[U^*], \Gamma_U^{\mathcal{E},\mathcal{D}}) \times d + 1}{d+1}, \tag{2.20}$$

where the integration is taken in the normalised Haar measure dU' [67].

where dU is the normalised Haar measure (see footnote 2 of Chap. 4 for the definition), is equal to

$$\frac{2}{d(d-1)}. \tag{2.22}$$

Here the maximisation is taken over all the pairs $\mathcal{E}$ and $\mathcal{D}$, and hence the quantity (2.22) gives the optimal approximation achievable by deterministically realisable supermaps.

In particular, the quantity (2.22) achieves to 1 when $d = 2$, and thus the unitary conjugation is deterministically and exactly realisable without replication when $d = 2$. This is a consequence of a well known relation

$$\sigma_y U \sigma_y = U^*, \tag{2.23}$$

for any SU(2) unitary U, where σ_y is the Pauli Y operator $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. This equation implies

$$\mathcal{U}[U^*] = \mathcal{U}[\sigma_y] \circ \mathcal{U}[U] \circ \mathcal{U}[\sigma_y], \tag{2.24}$$

for any 2-dimensional unitary U. Thus unitary conjugation is realisable by choosing encoder and decoder so that $\mathcal{E} = \mathcal{D} = \mathcal{U}[\sigma_y]$ for $d = 2$.

2.3 Conjugation induced quantities and their computation

In this section, we review several functions of quantum states defined by using an antiunitary operator, namely conjugation. We call them *conjugation induced quantities*. These quantities are used to characterise resources such as entanglement and asymmetries of states. As mentioned in the introduction, an implementation of state and channel transposition helps computation of conjugation induced measures.

We start from an introduction of the conjugation operator and summarise the equivalence of the transposition and conjugation in Sec. 2.3.1. After giving a short introduction to entanglement and the Schmidt coefficients in Sec. 2.3.2, we review definitions of several conjugation induced quantities in Sec. 2.3.3. We construct observables for these conjugation induced quantities in Chap. 4. Finally we review methods proposed to compute these conjugation induced quantities in Sec. 2.3.4. These methods provides us a motivation to investigate realisability of state and channel transpositions in Chaps. 3 and 4.

2.3.1 Antiunitary and transposition

Antiunitary transformations are closely related to a particular positive linear map, transposition. In this subsection, we review the connection between these two and their individual use in quantum physics.

An operator K on $\mathcal{H}$ is called antilinear if

$$K(a_1|\psi_1\rangle + a_2|\psi_2\rangle) = a_1^* K|\psi_1\rangle + a_2^* K|\psi_2\rangle, \tag{2.25}$$

holds for any vectors $|\psi_1\rangle$, $|\psi_2\rangle \in \mathcal{H}$ and complex coefficients a_1, $a_2 \in \mathbb{C}$. If an antilinear operator on $\mathcal{H}$ coincides with a complex conjugation in a basis of $\mathcal{H}$, it is called a *conjugation*. We denote a conjugation of interest by Θ. In this thesis, the complex conjugation for Θ is always taken in the computational basis, which coincides with the basis of transposition. Any other conjugation uniquely decomposes as $V\Theta$, where V is a unitary operator on $\mathcal{H}$ with $V = V^{\mathrm{T}}$. Any antilinear operator on $\mathcal{H}$ that is decomposable as $U\Theta$ with some unitary operator is called antiunitary.

Antiunitary operators do not describe a state evolution in the standard quantum physics. They appear in the form of fundamental symmetry transformations in particle physics such as time-reversal and charge-conjugation [9].

At the level of operators, antiunitary operators cannot act with unitary operators in parallel. Namely, if one tries to define $\Theta \otimes U$ so that $(\Theta \otimes U)|\psi\rangle \otimes |\phi\rangle = \Theta|\psi\rangle \otimes U|\phi\rangle$ holds for any product state vectors, it is easily noticed that its action on $(i|\psi\rangle) \otimes |\phi\rangle = |\psi\rangle \otimes (i|\phi\rangle)$ is not well defined. Symmetry transformations such as partial time-reversal and partial charge-conjugation are unphysical and more problematically, undefinable on product state vectors.

The adjoint action of antiunitary operators is, however, well-defined on a part of any bipartite Hermitian operators. Essentially it suffices to consider the action of $\mathcal{U}[\Theta]$ on parts of quantum systems, since the adjoint actions of any antiunitary operators decompose into $\mathcal{U}[U\Theta] = \mathcal{U}[U] \circ \mathcal{U}[\Theta]$. For a Hermitian operator $O \in \mathcal{B}(\mathcal{H})_{\mathrm{sa}}$, its action is

$$\mathcal{U}[\Theta](O) = \Theta O \Theta = O^* \Theta\Theta = O^* = O^{\mathrm{T}}, \tag{2.26}$$

where O^* represents the complex conjugation of O in the basis $\{|i\rangle\langle j|\}$. The last equality holds since O is Hermitian. Thus the adjoint action of conjugation operator $\mathcal{U}[\Theta]$ on Hermitian operators (including quantum states) coincides with transposition. For bipartite product Hermitian operators, its action on part of the system is well-defined:

$$\mathcal{U}[\Theta] \otimes \mathrm{id}_{\mathcal{K}}(O_{\mathcal{H}} \otimes O_{\mathcal{K}}) = O_{\mathcal{H}}^* \otimes O_{\mathcal{K}}. \tag{2.27}$$

Any bipartite Hermitian operator $O \in \mathcal{B}(\mathcal{H} \otimes \mathcal{K})$ decomposes into $O = \sum_i A_i \otimes B_i$ with Hermitian operators A_i on $\mathcal{H}$ and B_i on $\mathcal{K}$. An extension of Eq. (2.27) to bipartite Hermitian operators by

$$\mathcal{U}[\Theta] \otimes \mathrm{id}_{\mathcal{K}}(O) := \sum_i A_i^* \otimes B_i \tag{2.28}$$

is well-defined, since for any other decomposition $O = \sum_j C_j \otimes D_j$,

$$\sum_j C_j^* \otimes D_j = \sum_j C_j^{\mathrm{T}} \otimes D_j = O^{\mathrm{T}_{\mathcal{H}}} = \sum_i A_i^{\mathrm{T}} \otimes B_i' = \sum_i A_i^* \otimes B_i,$$

where $\mathrm{T}_{\mathcal{H}}$ represents the partial transposition on $\mathcal{H}$. Thus it is possible to define the action of $\mathcal{U}[\Theta]$ on parts of Hermitian operators, and it coincides with the partial transposition.

In general, conjugation $\mathcal{U}[\Theta]$ and transposition T differ in that the latter satisfies full linearity in complex coefficients. Nevertheless they coincide on the Hermitian operators, and this enables us to apply our investigations on state and channel transposition to computation of conjugated induced quantities reviewed in Sec. 2.3.3 (see Sec. 2.3.4 for more details).

2.3.2 Entanglement and Schmidt coefficients

In this subsection, we introduce the Schmidt decomposition of pure bipartite states and its relation to entanglement. The Schmidt coefficients are used to represent several conjugation induced quantities explicitly shown in Sec. 2.3.3. We also introduce a family of quantity defined with the Schmidt coefficients for which we find an alternative expression in Chap. 4.

A pure bipartite state $|\psi\rangle \in \mathcal{H} \otimes \mathcal{K}$ is said to be entangled if it is not a product of pure states in $\mathcal{H}$ and $\mathcal{K}$. The following set of coefficients characterises bipartite pure states.

Theorem 6 (Schmidt decomposition)**.** Let $|\psi\rangle$ be a pure state on $\mathcal{H} \otimes \mathcal{K}$, and $d := \min\{\dim \mathcal{H}, \dim \mathcal{K}\}$. There are sets of orthogonal pure states $\{|\phi_i^{\mathcal{H}}\rangle\}_{i=1,\ldots,d}$ on $\mathcal{H}$ and $\{|\phi_i^{\mathcal{K}}\rangle\}_{i=1,\ldots,d}$ on $\mathcal{K}$ such that $|\psi\rangle$ decomposes into

$$|\psi\rangle = \sum_{i}^{d} \sqrt{\lambda_i} |\phi_i^{\mathcal{H}}\rangle \otimes |\phi_i^{\mathcal{K}}\rangle, \tag{2.29}$$

with non-negative real numbers λ_i $(i = 1, ..., d)$ satisfying $\sum_i \lambda_i = 1$. The non-negative numbers λ_i $(i = 1, ..., d)$ are called the Schmidt coefficients of $|\psi\rangle$, and the number of positive Schmidt coefficients is called the Schmidt number. There exists a pair of unitary operators U on $\mathcal{H}$ and V on $\mathcal{K}$ such that $|\psi'\rangle = U \otimes V|\psi\rangle$ if and only if the Schmidt coefficients of $|\psi\rangle$ and $|\psi'\rangle$ coincide.

If an equivalence relation of the bipartite pure states is defined so that $|\psi\rangle \sim |\psi'\rangle$ when there is a local unitaries U on $\mathcal{H}$ and V on $\mathcal{K}$ mapping one to the other so that $U \otimes V|\psi\rangle = |\psi'\rangle$, the equivalence classes are completely characterised by the Schmidt coefficients.

Pure state entanglement is completely characterised by the Schmidt coefficients. Entanglement is a generic name for correlations that multipartite non-separable quantum state have[3]. Entanglement is usually considered to be independent on the specific choice of basis on local systems in a multipartite system, and is thus invariant under local unitary transformations. Entanglement of bipartite pure states is determined by Schmidt coefficients since it defines the equivalence classes through local unitary transformations. For example, several entanglement measures on bipartite states reduce to the entanglement entropy for pure states,

[3]Quantum states are said to be separable if it does not decompose into convex mixture of product states.

which is expressed by $-\sum_i \lambda_i \log_2 \lambda_i$ with the Schmidt coefficients. See e.g. [68] for more details on entanglement.

Any invertible function of the set of Schmidt coefficients as well characterise the equivalence classes. The analysis in Chap. 4 involves a family of quantities $\{\mathrm{C}_k^G\}_{k=1,\dots,d}$ defined by

$$\mathrm{C}_k^G(\psi) = d\left(\binom{d}{k} \sum_{i_1<\dots<i_k} \lambda_{i_1}\dots\lambda_{i_k}\right)^{-k}, \tag{2.30}$$

for bipartite pure state $|\psi\rangle \in \mathbb{C}_d \otimes \mathbb{C}_d$ with the Schmidt coefficients λ_i ($i = 1,\dots,d$) [69]. Here $\binom{d}{k}$ represents the binomial coefficient. The last one in this family $\mathrm{C}_d^G(\psi) = d\,(\lambda_1\dots\lambda_d)^{-d}$ is called G-concurrence[4]. The G-concurrence has an operational meaning with regard to a protocol called remote entanglement distribution [70, 69].

This family $\{\mathrm{C}_k^G\}_{k=1,\dots,d}$ completely characterises the bipartite pure state entanglement in the sense that the Schmidt coefficients are recoverable from the family. The family is easily computed from the description of pure state $|\psi\rangle$, without finding the values of the Schmidt coefficients. Observables for directly measuring the family $\{\mathrm{C}_k^G\}_{k=1,\dots,d}$ without requiring the recourse for state tomography have been found in Ref. [71] (see Sec. 2.3.4 for details). Our analysis on the unitary conjugation in Chap. 4 leads the same observables.

2.3.3 Conjugation induced quantities

In this section, we review several important quantities defined by using conjugation operators. A conjugation induced quantity called *concurrence* was first considered for bipartite entanglement in 2×2-dimensional system. Then several works followed to generalise the concurrence to higher-dimensional systems and multipartite systems. These generalised quantities are sometimes defined without using conjugation. More recently, the conjugation is used to quantify antiunitary asymmetries. Our review is restricted to quantities on pure states.

Concurrence The concurrence is first considered for bipartite 2-level states [72, 73]. For pure state $|\psi\rangle \in \mathbb{C}_2 \otimes \mathbb{C}_2$, the concurrence C is defined by

$$\mathrm{C}(\psi) := |\langle\psi|\sigma_y \otimes \sigma_y \Theta|\psi\rangle|. \tag{2.31}$$

The concurrence is invariant under local unitary transformations, and thus can be expressed in terms of the Schmidt coefficients of the pure state. If a pure bipartite qubit state $|\psi\rangle$ has Schmidt coefficients $\lambda_1,\ \lambda_2$ ($\lambda_1 + \lambda_2 = 1$) then

$$\mathrm{C}(\psi) = \lambda_1\lambda_2. \tag{2.32}$$

Much effort is devoted to generalise the concurrence to higher dimensions. The family $\{\mathrm{C}_k^G\}_{k=1,\dots,d}$ defined by Eq. (2.30) is obtained in this direction. Note that $(\mathrm{C}_2^G)^2/4$ coincides with concurrence when $d = 2$. The following two are examples obtained in the same direction.

[4]The initial G for G-concurrence stands for “geometric”.

Θ-concurrence In Ref. [74], Uhlmann extends the definition of the concurrence straightforwardly to higher dimensions, and calls it Θ-concurrence. This quantity is defined without pre-existing partitioning of the Hilbert space $\mathcal{H}$ while bipartition is required for defining the concurrence. Because of this property, the Θ-concurrence does not necessarily characterise entanglement. For a pure state $\psi \in \mathcal{H}$, Θ-concurrence C_Θ is defined by

$$\mathrm{C}_\Theta(\psi) := |\langle\psi|\Theta|\psi\rangle|, \tag{2.33}$$

and depends on the basis in which Θ represents the complex conjugation. It does not coincide with the concurrence for $2 \times 2 = 4$-dimensional systems.

***I*-concurrence** Contrary to the Θ-concurrence, the I-concurrence presented in Ref. [75] is invariant under local unitary channels, and characterises multipartite correlation. We rewrite the pure state concurrence (2.31) as

$$\sqrt{\langle\psi|S_2 \otimes S_2(|\psi\rangle\langle\psi|)|\psi\rangle}, \tag{2.34}$$

where $S_2 : \mathcal{B}(\mathbb{C}_2) \to \mathcal{B}(\mathbb{C}_2)$ is the positive map given by

$$S_2 = \mathcal{U}[\sigma_y] \circ \mathcal{U}[\Theta]. \tag{2.35}$$

Their starting point is the observation that the pure state concurrence is invariant under local unitary channels since $S_2 \circ \mathcal{U}[U] = \mathcal{U}[U] \circ S_2$ holds for any unitary operator U on $\mathbb{C}_2$. If there exists a map $S_d : \mathcal{B}(\mathbb{C}_d) \to \mathcal{B}(\mathbb{C}_d)$ such that

$$S_d \circ \mathcal{U}[U] = \mathcal{U}[U] \circ S_d, \tag{2.36}$$

for any unitary operator U on $\mathbb{C}_d$, then it may be used to define a local unitary invariant on higher dimensional systems (see Eq. (2.38)). We generalise Eq. (2.36) to obtain our unitary conjugation scheme in Chap. 4. With several other natural requirements for S_d, the authors show that S_d must be the universal inverter defined by

$$S_d := \nu_d \sum_{1 \le j < k \le d} \mathcal{U}[\frac{-i}{\sqrt{2}}(|j\rangle\langle k| - |k\rangle\langle j|)] \circ \mathrm{T}, \tag{2.37}$$

where ν_d is a positive constant. The I-concurrence C_I of a pure state $|\psi\rangle$ on a $d_1 \times d_2$ dimensional system is defined by

$$\begin{aligned} \mathrm{C}_I(\psi) &= \sqrt{\langle\psi|S_{d_1} \otimes S_{d_2}(|\psi\rangle\langle\psi|)|\psi\rangle} && (2.38)\\ &= \sqrt{2\nu_{d_1}\nu_{d_2}(1 - \mathrm{Tr}[(\mathrm{Tr}_A[|\psi\rangle\langle\psi|])^2])} \\ &= 2\sqrt{\nu_{d_1}\nu_{d_2}\sum_{i<j}\lambda_i\lambda_j}, && (2.39) \end{aligned}$$

where λ_i $(i = 1, ..., \min\{d_1, d_2\})$ are the Schmidt coefficients. The I-concurrence is proportional to the second of the family $\{\mathrm{C}_k^G\}_{k=1,...,d}$ defined by Eq. (2.30).

Filter based quantities So far we have reviewed extensions of the concurrence to higher dimensions characterising bipartite correlations (except the Θ-concurrence, whose physical interpretation is missing). A quantity measuring tripartite entanglement called 3-tangle (or "three-way tangle" in their original paper) was first defined in terms of coefficients of tripartite pure states [76]. Later, alternative expressions of 3-tangle using conjugation were found in Ref. [77]. 3-tangle τ_3 of a pure tripartite state $|\psi\rangle \in \mathbb{C}_2 \otimes \mathbb{C}_2 \otimes \mathbb{C}_2$ is

$$\tau_3(\psi) = |g^{\mu\nu}\langle\psi|\sigma_\mu \otimes \sigma_y \otimes \sigma_y \Theta|\psi\rangle\langle\psi|\sigma_\nu \otimes \sigma_y \otimes \sigma_y \Theta|\psi\rangle|, \tag{2.40}$$

where sumamtion is taken for indices $\mu,\ \nu \in \{0,1,2,3\}$, and $\sigma_0 = \mathbb{I}_2$, $\sigma_1 = \sigma_x$, $\sigma_2 = \sigma_y$, $\sigma_3 = \sigma_z$ and $g = \mathrm{diag}(-1,1,0,1)$.

In Ref. [77], a method to construct multipartite entanglement monotones is presented. It starts from a building block called a "comb" (note that this comb is different from those representing supermaps). A comb of order n is an operator O on $\mathbb{C}_2^{\otimes n}$ satisfying

$$\langle\psi|^{\otimes n} O\Theta|\psi\rangle^{\otimes n} = 0 \tag{2.41}$$

for any pure state $\psi \in \mathbb{C}_2$. The only non-trivial first order comb is known to be σ_y ($O = 0$ is the trivial comb). The operator $g^{\mu\nu}\sigma_\mu \bullet \sigma_\nu$ on $\mathbb{C}_2 \otimes \mathbb{C}_2$ is a comb of second order, where we distinguish the tensor product between clones from that between partitions of system, and denote it by $\bullet$ in this thesis. Once we have combs, multipartite entanglement monotones are defined as expectation values of operators called "filters". Filters for n partite systems are tensor products of n combs preceded by conjugation. For example, the concurrence is defined by a filter

$$\sigma_y \otimes \sigma_y \Theta. \tag{2.42}$$

3-tangle has two different equivalent filters

$$g^{\mu\nu}(\sigma_\mu \otimes \sigma_y \otimes \sigma_y) \bullet (\sigma_\nu \otimes \sigma_y \otimes \sigma_y)\Theta, \text{ and} \tag{2.43}$$

$$\frac{1}{3} g^{\mu_1\nu_1} g^{\mu_2\nu_2} g^{\mu_3\nu_3} (\sigma_{\mu_1} \otimes \sigma_{\mu_2} \otimes \sigma_{\mu_3}) \bullet (\sigma_{\nu_1} \otimes \sigma_{\nu_2} \otimes \sigma_{\nu_3})\Theta, \tag{2.44}$$

where in this case expectation values are taken with cloned states $|\psi\rangle \bullet |\psi\rangle$ ($|\psi\rangle \in \mathbb{C}_2 \otimes \mathbb{C}_2 \otimes \mathbb{C}_2$). This method can construct n-qubit entanglement monotones where n is arbitrary.

Antiunitary asymmetries Resource theories of asymmetry aims at quantifying how a resource state deviates from those states with a given symmetry. Resource theories of antiunitary asymmetries in particular quantify violation of symmetries represented by antiunitary transformations such as time-reversal and charge conjugation. Among many different formulations, we here review the resource theory of special antiunitary asymmetry proposed in Ref. [39].

The antiunitary operator representing the symmetry is $P\Theta$ where P is a unitary operator on $\mathcal{H}$ satisfying $P^\dagger = P$, $P^2 = \mathbb{I}_\mathcal{H}$, and $P\Theta = \Theta P$. These conditions implies $(P\Theta)^\dagger = P\Theta$. A state $\rho \in \mathcal{S}(\mathcal{H})$ is said to be $\mathcal{PT}$-symmetric if $\mathcal{U}[P\Theta](\rho) = \rho$. The set of all $\mathcal{PT}$-symmetric states is denoted by $\mathrm{Sym}(\mathcal{PT})$. The violation of $\mathcal{PT}$-symmetry is quantified by several different quantities which give zero for $\mathcal{PT}$-symmetric states. This thesis treats two $\mathcal{PT}$-asymmetry measures presented there.

- The skew information of $\mathcal{PT}$-asymmetry Γ_s is defined by

$$\Gamma_s(\rho) := -\frac{1}{2}\mathrm{Tr}[[\rho, P\Theta]^2]. \tag{2.45}$$

For pure states, this reduces to

$$\Gamma_s(|\psi\rangle\langle\psi|) = 1 - |\langle\psi|P\Theta|\psi\rangle|^2. \tag{2.46}$$

- The fidelity measure of $\mathcal{PT}$-asymmetry is defined by

$$\Gamma_F(\rho) := 1 - \mathrm{Tr}[\sqrt{\sqrt{\rho}P\Theta\rho P\Theta\sqrt{\rho}}]. \tag{2.47}$$

For pure states, this reduces to

$$\Gamma_F(|\psi\rangle\langle\psi|) = 1 - |\langle\psi|P\Theta|\psi\rangle|. \tag{2.48}$$

Reference [39] also proposes a method to measure these two quantities for pure states. We review their method with other existing methods to compute conjugation induced quantities in the following subsection.

2.3.4 Computation of conjugation induced quantities

There are several methods to calculate quantities listed in the previous subsection even in the case where descriptions of states are not given. Some of them use the fact that these quantities are induced by conjugation.

Of course it is possible to obtain the description of an unknown state by performing tomography if we have sufficiently many clones of the unknown state. Once we obtain the description of the state, we can calculate any quantities by classical computer. All the methods listed below are more efficient in some sense compared to the methods via tomography and classical computation.

Embedding quantum simulators An embedding quantum simulator is a devise that simulates a quantum system (called a simulated space) by an enlarged quantum system (called a simulating space). The embedding quantum simulator for antilinear transformations is proposed in Ref. [40].

For simulating a system described by Hilbert space $\mathcal{H} = \mathbb{C}_d$, it uses a space $\mathbb{C}_2 \otimes \mathcal{H}$ that is enlarged by a qubit system. Let $(\psi_1\ \psi_2\ ...\ \psi_d)^{\mathrm{T}}$ be the state vector for $|\psi\rangle$ decomposed in the basis for conjugation, and O be an operator on $\mathcal{H}$. Then define a mapping $\underline{\mathrm{Maj}}$ by

$$\underline{\mathrm{Maj}} : |\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_d \end{pmatrix} \quad \mapsto \quad |\psi\rangle_{sim} := \frac{1}{2}\begin{pmatrix} \psi_1 + \psi_1^* \\ \vdots \\ \psi_d + \psi_d^* \\ -i(\psi_1 - \psi_1^*) \\ \vdots \\ -i(\psi_d - \psi_d^*) \end{pmatrix} \tag{2.49}$$

for states, and

$$\underline{\mathrm{Maj}} : O \quad \mapsto \quad O_{sim} := \mathbb{I}_2 \otimes \frac{1}{2}(O + \Theta O \Theta) - i\sigma_y \otimes \frac{-i}{2}(O - \Theta O \Theta), \quad (2.50)$$

for operators. The inverse of mapping $\underline{\mathrm{Maj}}$ on states (2.49) is presented by an operator $M := (1\ i) \otimes \mathbb{I}_d$. For a unitary operator U and an Hermitian operator H on $\mathcal{H}$, U_{sim} and H_{sim} are also unitary and Hermitian, respectively, and

$$U|\psi\rangle \mapsto U_{sim}|\psi\rangle_{sim}, \quad (2.51)$$

$$\exp(-iHt) \mapsto \exp(-iH_{sim}t) \quad (2.52)$$

hold. The corresponding unitary channel $\mathcal{U}[U] = \mathcal{U}[\exp(-iHt)]$ on $\mathcal{H}$ is simulated by the unitary channel $\mathcal{U}[U_{sim}] = \mathcal{U}[\exp(-iH_{sim}t)]$.

Although conjugation $|\psi\rangle \mapsto |\psi^*\rangle$ is an antiunitary transformation, it is simulated by a unitary channel $\mathcal{U}[\sigma_z \otimes \mathbb{I}_d]$ in the sense $|\psi^*\rangle_{sim} = \sigma_z \otimes \mathbb{I}_d|\psi\rangle_{sim}$. In other words, the following diagram commutes:

$$\begin{array}{ccc} |\psi\rangle & \xrightarrow{\Theta} & |\psi^*\rangle \\ \downarrow{\scriptstyle \underline{\mathrm{Maj}}} & & \downarrow{\scriptstyle \underline{\mathrm{Maj}}} \\ |\psi\rangle_{sim} & \xrightarrow{\sigma_z \otimes \mathbb{I}_d} & |\psi^*\rangle_{sim}. \end{array}$$

The simulation of time-reversal and charge conjugation has already been demonstrated in an experiment [78].

Embedding quantum simulators are theoretically shown to be useful for computation of several entanglement measures [38]. Let us consider a task to estimate some entanglement measure for state $|\psi_{fin}\rangle := \exp(-iH)|\psi_{init}\rangle$ under an assumption that descriptions of initial state $|\psi_{init}\rangle \in \mathcal{H}$ and Hamiltonian H is given. The task is straightforwardly accomplished by calculating the description of $|\psi_{fin}\rangle$ from those of $|\psi_{init}\rangle$ and H, but this calculation may be very hard when the system size is very large and it is difficult to diagonalise H.

Another way to accomplish the task is provided by quantum simulators. By creating the state $|\psi_{init}\rangle$ and performing Hamiltonian dynamics $\exp(-iH)$ in the simulator, we obtain the final state $|\psi_{fin}\rangle$. By repeating this step many times, we obtain the description of state $|\psi_{fin}\rangle$ by performing tomography on the clones without diagonalising H.

Several measures induced by conjugation can be calculated without requiring the recourse for the tomography, by using embedding quantum simulators [38]. Let us consider expectation value

$$\langle\psi_{fin}|O\Theta|\psi_{fin}\rangle \quad (2.53)$$

for an operator O on simulated space $\mathcal{H}$. Note that the concurrence, Θ-concurrence, I-concurrence, 3-tangle and its n-qubit generalisations for pure states can all be expressed in terms of the expectation value (2.53) for certain (possibly sets of) operators O. The expectation value (2.53) can be rewritten into

$$\langle\psi_{fin}|_{sim} M^\dagger O M |\psi^*_{fin}\rangle_{sim} \quad = \quad \langle\psi_{fin}|_{sim} M^\dagger O M \sigma_z \otimes \mathbb{I}_d |\psi_{fin}\rangle_{sim} \quad (2.54)$$

$$= \quad \langle\psi_{fin}|_{sim} (\sigma_z - i\sigma_x) \otimes O |\psi_{fin}\rangle_{sim}, \quad (2.55)$$

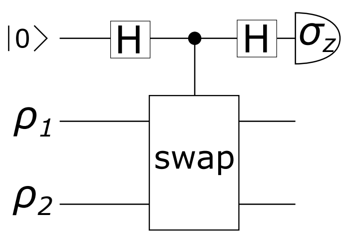

Figure 2.1: A quantum circuit to estimate the overlap $\mathrm{Tr}[\rho_1\rho_2]$ between two states ρ_1 and ρ_2 both in $\mathcal{S}(\mathcal{H})$. The lower two wires represent identity channels on $\mathcal{H}$, while upper one represents identity channel on a 2-dimensional space. The boxes labelled H, SWAP and σ_z represent the Hadamard gate, the controlled-swap gate, and the measurement in the computational basis $\{|0\rangle, |1\rangle\}$, respectively.

where the second equality follows from $M^\dagger O M \sigma_z \otimes \mathbb{I}_d = (\sigma_z - i\sigma_x) \otimes O$. Thus an expectation value of an antilinear operator in the simulated space corresponds to that of a linear operator in the simulating space. Moreover, Eqs. (2.51) and (2.52) imply that the final state $|\psi_{fin}\rangle_{sim}$ in the simulating space can be obtained by creating $|\psi_{init}\rangle_{sim}$ and transforming it by $\exp(-iH_{sim})$.

In summary, the expectation value (2.53) is obtained without tomography of $|\psi_{fin}\rangle$ by creating $|\psi_{init}\rangle_{sim}$, transforming it by Hamiltonian dynamics of H_{sim}, measuring expectation values of several observables in the simulated space so that the expectation value of $(\sigma_z - i\sigma_x) \otimes O$ is calculable from them. Compared to the method via tomography, the number of measurement settings (corresponding to the number of observables) required for calculating several entanglement measures such as the concurrence and the filter based measures is reduced by this method.

For implementing the mapping $\underline{\mathrm{Maj}}$, it is implicitly assumed that the descriptions of the state and Hamiltonian are given. It is already pointed out in Ref. [38] that the mapping $\underline{\mathrm{Maj}}$ is not physically realisable on unknown states and operators.

Direct estimation of overlaps between states Let us consider a task to calculate the absolute value of the expectation value (2.53) for the state $|\psi_{fin}\rangle := \exp(-iH)|\psi_{init}\rangle$ where descriptions of the initial state $|\psi_{init}\rangle \in \mathcal{H}$ and Hamiltonian H are given. When O is a unitary operator, an embedding quantum simulator and method proposed in Ref. [79] can be combined to accomplish this task [39].

For two unknown states ρ_1 and ρ_2, their overlap

$$\mathrm{Tr}[\rho_1\rho_2] \tag{2.56}$$

is calculable by applying the operation given by the quantum circuit presented in Fig. 2.1 [79]. If the probability to find the qubit in state $|0\rangle$ in the σ_z-measurement is p_0,

$$p_0 = \frac{1}{2}(1 + \mathrm{Tr}[\rho_1\rho_2]^2). \tag{2.57}$$

holds.

The absolute value of the expectation value (2.53) is the square root of the overlap between $\rho_1 = O|\psi_{fin}\rangle\langle\psi_{fin}|O^\dagger$ and $\rho_2 = |\psi^*_{fin}\rangle\langle\psi^*_{fin}|$. State $\mathcal{U}[O](|\psi_{fin}\rangle\langle\psi_{fin}|)$

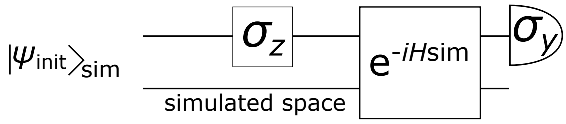

Figure 2.2: A quantum circuit to produce state $\Theta|\psi_{fin}\rangle = \Theta\left(\exp(-iH)|\psi_{init}\rangle\right)$. The lower wire represents the identity channel on the simulated space $\mathcal{H}$, while the upper one represents the identity channel on a 2-dimensional system. The boxes labelled σ_z, $\exp(-iH_{sim})$, and σ_y stands for the σ_z-gate, unitary channel $\mathcal{U}[\exp(-iH_{sim})]$, and the measurement in eigenbasis of σ_y.

is obtained by applying the unitary channel $\mathcal{U}[O]$ on $|\psi_{fin}\rangle\langle\psi_{fin}|$. State $|\psi^*_{fin}\rangle\langle\psi^*_{fin}|$ is probabilistically obtained by first creating $|\psi_{init}\rangle_{sim}$ in the embedding quantum simulator, transforming it to $|\psi_{fin}\rangle_{sim} = \exp(-iH_{sim})|\psi_{init}\rangle_{sim}$ by Hamiltonian dynamics of H_{sim}, and then performing a measurement in the σ_y basis on the ancillary qubit (see Fig. 2.2). If the result of the σ_y measurement suggests $\sigma_y = -1$ (equivalently, if the qubit state is $(1\ i)^\dagger$), then the resulting state is $|\psi^*_{fin}\rangle\langle\psi^*_{fin}|$.

In summary, the absolute value of the expectation (2.53) is computed by first creating states $O|\psi_{fin}\rangle\langle\psi_{fin}|O^\dagger$ and $|\psi^*_{fin}\rangle\langle\psi^*_{fin}|$ with an embedding quantum simulator, and then estimating the overlap between these two states by using the quantum circuit presented in Fig. 2.1. The idea to combine embedding quantum simulator and the direct estimation of state overlaps is first proposed in Ref. [39] for estimating special antiunitary asymmetries.

The methods for computation of entanglement reviewed in Secs. 2.3.4 and 2.3.4 are guaranteed to work under the assumption that the descriptions of the initial state $|\psi_{init}\rangle$ and Hamiltonian H are given, since these methods utilise the embedding quantum simulator. For applying the direct estimation of state overlaps, it suffices if we could create the conjugated states by any methods like embedding quantum simulators. It is still not known if the description of the unknown state is *required* for creating its conjugation. Reducing the resource required for creating the conjugated states would help computing the conjugation induced quantities. Our investigation on chapters 3 and 4 are motivated from this observation.

Observable entanglement measures Several entanglement measures are calculated directly as expectation values of observables, and called observable entanglement measures for this reason. Most generally, observables for measuring local unitary invariants are considered, independently to conjugation induced quantities. Observables for specific conjugation induced quantities are considered in, for example, Refs. [80, 71, 81].

Reference [81] presented a method to construct observables for any filter based measures. Although the method is mainly aimed at constructing filter based $\mathrm{SL}(2,\mathbb{C})$-invariant quantities on mutipartite qubit systems, it can be applied most generally to quantities decomposed into elements with the form

$$\langle\psi|O|\psi^*\rangle\langle\psi^*|O^\dagger|\psi\rangle \tag{2.58}$$

with an Hermitian operator O. All the examples of conjugation induced quantities presented in the previous subsection are decomposable to elements of this form.

The element (2.58) is transformed into

$$\langle\psi|^{\bullet 2}\mathrm{T}_{\mathcal{H}}\bullet\mathrm{id}_{\mathcal{H}}(O\bullet O\ \mathrm{SWAP}_{\mathcal{H}\bullet\mathcal{H}})|\psi\rangle^{\bullet 2}, \tag{2.59}$$

where we use symbol $\bullet$ to represent the tensor product between cloned states. The operator $\mathrm{SWAP}_{\mathcal{H}\bullet\mathcal{H}}=\sum_{i,j=1}^{\dim\mathcal{H}}(|i\rangle\bullet|j\rangle)(\langle j|\bullet\langle i|)$ represents the swap operator between clones. The Hermitian operator

$$\mathrm{T}_{\mathcal{H}}\bullet\mathrm{id}_{\mathcal{H}}(O\bullet O\ \mathrm{SWAP}_{\mathcal{H}\bullet\mathcal{H}}) \tag{2.60}$$

is the observable on cloned states to measure element (2.58).

References [82, 83] also presents a relation between conjugation induced quantities and their observables. Let $\Gamma:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{H})$ be a CP map whose input and the output Hilbert spaces have the same dimension, and $\Gamma(\cdot)=\sum_i T_i\cdot T_i^\dagger$ be the Kraus decomposition. Based on an equation

$$\langle\psi_1\otimes\psi_2|\widetilde{\Gamma}|\psi_3\otimes\psi_4\rangle=\sum_i\langle\psi_2|T_i|\psi_4^*\rangle\langle\psi_1^*|T_i^\dagger|\psi_3\rangle \tag{2.61}$$

shown in Ref. [82] for the Choi operator $\widetilde{\Gamma}$ of Γ, they observes

$$\langle\psi\otimes\psi|\widetilde{\Gamma}|\psi\otimes\psi\rangle=\sum_i|\langle\psi|T_i\Theta|\psi\rangle|^2. \tag{2.62}$$

Note that all the conjugation induced quantities reviewed in Sec. 2.3.3 except the filter-based quantities can be represented in the form of the right hand side of Eq. (2.62) with the appropriate choices of the Kraus operators. Once decomposed into the form presented by Eq. (2.58), the filter-based quantities can be represented by the product of the right hand side of Eq. (2.62).

In Ref. [80], Mintert considers observables on cloned states that induce bipartite local unitary invariants. Let us consider bipartite states on $\mathcal{H}_A\otimes\mathcal{H}_B$, and denote tensor products of the bi-partition by $\otimes$ and those on clones by $\bullet$, as we have introduced when dealing with filter-based quantities. If O is an observable on $(\mathcal{H}_A\otimes\mathcal{H}_B)^{\bullet n}$ satisfying

$$O=U_A^{\dagger\bullet n}\otimes U_B^{\dagger\bullet n}OU_A^{\bullet n}\otimes U_B^{\bullet n}, \tag{2.63}$$

for any unitary operators U_A and U_B on $\mathcal{H}_A$ and $\mathcal{H}_B$, then

$$\langle\psi|^{\bullet n}O|\psi\rangle^{\bullet n}, \tag{2.64}$$

for state $|\psi\rangle\in\mathcal{H}_A\otimes\mathcal{H}_B$, is clearly invariant under local unitary channels. Mintert constructs observables satisfying Eq. (2.63) such that expectation values (2.64) coincide with concurrence, 3-tangle and the G-concurrence for 3×3 and 4×4 dimensional systems. Observables for G-concurrences on arbitrary $d\times d$ dimensional systems and the entire family $\{\mathrm{C}_k^G\}_{k=1,\dots,d}$ of the concurrence monotones are found by Oszmaniec [71]. He shows

$$\sqrt[k]{\langle\psi|^{\bullet k}\Pi_{\mathcal{H}^{\wedge k}}\otimes\Pi_{\mathcal{H}^{\wedge k}}|\psi\rangle^{\bullet k}}\propto\mathrm{C}_k^G(\psi), \tag{2.65}$$

where $\Pi_{\mathcal{H}^{\wedge k}}$ represents the projector onto the antisymmetric subspace of $\mathcal{H}^{\bullet k}$. The observable $\Pi_{\mathcal{H}^{\wedge k}} \otimes \Pi_{\mathcal{H}^{\wedge k}}$ satisfies Eq. (2.63), since the k-th antisymmetric subspace is invariant under the k collective actions of the unitary. However, Mintert's (and thus Oszmaniec's) method does not provide a prescription to construct observable entanglement measures for given quantities.

In summary, all the conjugation induced quantities presented in Sec. 2.3.3 find their corresponding observables by the method presented in Ref. [81] and Refs. [82, 83]. Observables for the filter-based quantities are also found in Ref. [80]. The family $\{\mathrm{C}_k^G\}_{k=1,\ldots,d}$ of concurrence monotones, defined without conjugation in Ref. [69], also find their observables [71] by the same approach from Ref. [80].

In Chap. 4, we show that the observables constructed by the methods presented in Ref. [81] and Refs. [82, 83] are equivalent, by proposing a more general and unified method which includes the two methods as particular cases. Our analysis on the unitary conjugation suggests expressions of the family $\{\mathrm{C}_k^G\}_{k=1,\ldots,d}$ as conjugation induced quantities, and the proposed method constructs the same observables for $\{\mathrm{C}_k^G\}_{k=1,\ldots,d}$ to those presented by Oszmaniec [71].

Chapter 3

Realisability of positive non-CP maps on states

In this chapter, we analyse the gap between positive and CP maps under the assumptions that input states are uncorrelated to other systems and the finitely cloned input states are available. As noted in the introduction, the finite clone assumption releases the linearity constraints of quantum theory and if infinitely many clones are available, the gap between positive and CP maps disappears. Although infinite clones of the unknown state are sufficient, they might not be necessarily for realising specific positive non-CP maps. That is, the gap between positive and CP maps may become close even with finite clones. We are interested in the behaviour of this gap, and investigate the number of clones required for performing several positive non-CP maps probabilistically.

Among all those positive non-CP maps, we pay a special attention to transposition. Besides of the fundamental interest, reducing the resource required for transposition is helpful for computation of several entanglement measures as discussed in the previous chapter (see Sec. 2.3.4 for details).

By using a result of preceding work reviewed in Sec. 2.1.2, we show that infinite clones are not only sufficient but also necessary for realising state transposition even probabilistically in Sec. 3.1. We also give an alternative proof of this fact for transpositions on $d \geq 3$-dimensional systems in Sec. 3.2. Although this alternative proof does not apply for 2-dimensional transposition, it covers the impossibility of other kind of positive non-CP maps than the transposition.

3.1 Necessity of infinite clones for probabilistic transposition

In this section we show that transposition on an unknown state is not probabilistically realisable if only finite clones of the state are given, even when the unknown input state is uncorrelated to other systems[1]. We say that transposition on Hilbert space $\mathcal{H}$ is probabilistically (deterministically) realisable from n-clones,

[1] A slightly generalised version of the no-go result presented in Sec. 3.1 is in Ref. [84]

if there exists a TNICP (TPCP) map $\mathcal{E} : \mathcal{B}(\mathcal{H}^{\otimes n}) \to \mathcal{B}(\mathcal{H})$ satisfying

$$\epsilon \leq \mathrm{Tr}[\mathcal{E}(\rho^{\otimes n})], \qquad \mathcal{E}(\rho^{\otimes n}) \propto \rho^{\mathrm{T}} \qquad (\forall \rho \in \mathcal{S}(\mathcal{H})), \tag{3.1}$$

for some positive real number $\epsilon > 0$. The success probability $\mathrm{Tr}[\mathcal{E}(\rho^{\otimes n})]$ may depend on the state ρ.

The difference between "deterministic approximate" and "probabilistic" realisations is worth noting here. Let us, for example, consider a TPCP map $\Gamma : \mathcal{B}(\mathbb{C}_2^{\otimes m}) \to \mathcal{B}(\mathbb{C}_2)$ that optimally approximates the universal-NOT transformation in the sense of Ref. [27] (see Sec. 2.1.2). Γ is "deterministic" in that it can be implemented with a unit probability. Γ "approximates" the universal-NOT transformation in that the output of Γ may be different from the target state $|\psi^\perp\rangle\langle\psi^\perp|$. On the other hand when we further require Γ to realise the universal-NOT transformation "probabilistically," then Γ must be represented by an instrument $\{\mathcal{E}_i : \mathcal{B}(\mathbb{C}_2^{\otimes m}) \to \mathcal{B}(\mathbb{C}_2)\}$ such that $\Gamma = \sum_i \mathcal{E}_i$ and $\mathcal{E}_i(|\psi\rangle\langle\psi|^{\otimes m}) \propto |\psi^\perp\rangle\langle\psi^\perp|$ for at least one of the outcomes $\{i\}$. Even if Γ optimally approximates the universal-NOT transformation, it does not necessarily realise the universal-NOT transformation probabilistically. In turn even if Γ probabilistically realise the universal-NOT transformation probabilistically, it may not be an optimal approximation.

Let us assume that a TNICP map $\mathcal{E} : \mathcal{B}(\mathbb{C}_2^{\otimes m}) \to \mathcal{B}(\mathbb{C}_2)$ realises probabilistic transposition on the 2-dimensional Hilbert space from finite m clones. We derive a contradiction to the optimal fidelity of universal-NOT transformation presented by Eq. (2.8).

There exists an another TNICP map $\mathcal{E}'$ such that $\{\mathcal{E},\ \mathcal{E}'\}$ forms an instrument. We denote the success probability of state transposition by

$$p_{|\psi\rangle} := \mathrm{Tr}[\mathcal{E}(|\psi\rangle\langle\psi|)], \tag{3.2}$$

which is assumed to be no less than a positive real number ϵ. Note that the minimum p might be very small but not zero since $0 < \epsilon \leq p$.

Now assume that $m \times l$ clones of the unknown state $|\psi\rangle\langle\psi|$ is given on space $\mathbb{C}_2^{\otimes m \times l}$. We label the 2-dimensional spaces $\mathbb{C}_2$ in ith ($i = 1, ..., l$) block of Hilbert space $\mathbb{C}_2^{\otimes m}$ by $\mathcal{H}_i$, and denote $\mathbb{C}_2^{\otimes m \times l}$ by $\bigotimes_{i=1}^{l} \mathcal{H}_i^{\otimes m}$, CP maps $\mathcal{E},\ \mathcal{E}'$ applied on the ith system by $\mathcal{E}_i,\ \mathcal{E}_i'$. We consider applying the following sequence of operations on the cloned states. First, perform instruments $\{\mathcal{E}_i,\ \mathcal{E}_i'\}$ on all the l blocks. If we know that this instrument "succeeded" for some i (meaning that $\mathcal{E}_i$ is performed on the ith system), then choose the state of the ith system as the output. If we do not succeeded in any i (meaning that $\mathcal{E}_i'$ is performed on all systems $i = 1, ..., l$), then output a state $|0\rangle\langle 0|$ (in this case we abort). The probability of not having success in any i is given by

$$(1 - p_{|\psi\rangle})^l. \tag{3.3}$$

For concreteness we show an explicit construction of the TPCP map presented by these sequence of operations. Other than the Hilbert spaces $\mathcal{H}_i$, we need ancillary systems $\mathcal{K}_i \cong \mathbb{C}_2$ for all i, and yet another ancillary system $\mathcal{H}$ whose state is initialised to $|0\rangle\langle 0|$. Figure 3.1 represents the quantum circuit representation of the

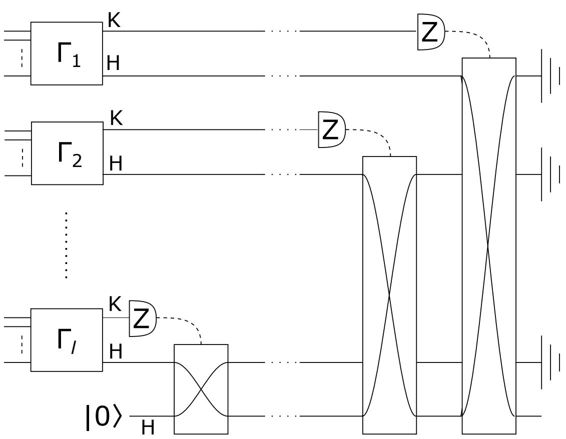

Figure 3.1: The quantum circuit representation of TPCP map Γ presented in Eq. (3.6). Boxes labelled Z represents measurements on computational basis $\{|0\rangle,\ |1\rangle\}$. The white boxes with crossing lines inside represent conditional swap operations applying SWAP bewteen Hilbert spaces corresponding to the crossing lines if the outcome of the measurements are 1 (otherwise they do nothing). The ground symbols represent partial traces on corresponding systems. The TPCP maps Γ_i' $(i = 1, ..., l)$ defined by Eq. (3.5) is presented here by swap operations conditioned on the measurement outcomes on $\mathcal{K}$.

TPCP map Γ we are going to construct. The first step of performing instruments $\{\mathcal{E}_i,\ \mathcal{E}_i'\}$ is presented by a TPCP map

$$\Gamma_i(\cdot) := \mathcal{E}_i(\cdot) \otimes |1\rangle\langle 1|_{\mathcal{K}_i} + \mathcal{E}_i'(\cdot) \otimes |0\rangle\langle 0|_{\mathcal{K}_i} \tag{3.4}$$

from $\mathcal{B}(\mathcal{H}_i^{\otimes m})$ to $\mathcal{B}(\mathcal{K}_i \otimes \mathcal{H}_i)$. It is a routine work to show that Γ_i is TPCP. The second step for choosing a success state is presented by a TPCP map

$$\Gamma_i' := \mathrm{id}_{\mathcal{H}_i \otimes \mathcal{H}} \otimes (\mathrm{Tr}_{\mathcal{K}_i} \circ \mathcal{U}[|0\rangle\langle 0|_{\mathcal{K}_i}]) + \mathrm{SWAP}_{\mathcal{H}_i, \mathcal{H}} \otimes (\mathrm{Tr}_{\mathcal{K}_i} \circ \mathcal{U}[|1\rangle\langle 1|_{\mathcal{K}_i}]) \tag{3.5}$$

from $\mathcal{B}(\mathcal{H} \otimes \mathcal{H}_i \otimes \mathcal{K}_i)$ to $\mathcal{B}(\mathcal{H} \otimes \mathcal{H}_i)$, where $\mathrm{SWAP}_{\mathcal{H}_i, \mathcal{H}}$ represents the swap operation between $\mathcal{H}_i$ and $\mathcal{H}$. Γ_i' does nothing if the state of the register $\mathcal{K}_i$ is 0 (corresponding to the failure), and swap the states on $\mathcal{H}$ and $\mathcal{H}_i$ if 1 (corresponding to the success). The composition

$$\Gamma := \mathrm{Tr}_{\otimes_i \mathcal{H}_i} \circ \Gamma_1' \circ ... \circ \Gamma_l' \circ \bigotimes_{i=1}^{l} \Gamma_i \circ (\cdot \otimes |0\rangle\langle 0|_{\mathcal{H}}), \tag{3.6}$$

where $(\cdot \otimes |0\rangle\langle 0|_{\mathcal{H}})$ creates state $|0\rangle\langle 0|$ on $\mathcal{H}$, represents the desired TPCP map.

If one obtains the success in any of l blocks, the state on $\mathcal{H}$ is swapped to the success state. Since the probability of not having the success in all i is given by Eq. (3.3),

$$\Gamma(|\psi\rangle\langle\psi|^{\otimes m \times l}) = (1 - (1 - p_{|\psi\rangle})^l)(|\psi\rangle\langle\psi|)^{\mathrm{T}} + (1 - p_{|\psi\rangle})^l |0\rangle\langle 0| \tag{3.7}$$

holds for any pure state $|\psi\rangle \in \mathbb{C}_2$.

Equation (3.7) implies

$$\begin{aligned} & \mathrm{Tr}[|\psi^\perp\rangle\langle\psi^\perp|\ \mathcal{U}[\sigma_y]\circ\Gamma(|\psi\rangle\langle\psi|^{\otimes m\times l})] && (3.8)\\ = & \ (1-(1-p_{|\psi\rangle})^l)+(1-p_{|\psi\rangle})^l\mathrm{Tr}[|\psi^\perp\rangle\langle\psi^\perp||1\rangle\langle 1|] && (3.9)\\ \geq & \ (1-(1-\epsilon)^l). && (3.10)\end{aligned}$$

For sufficiently large l, $\mathcal{U}[\sigma_y]\circ\Gamma$ realises the universal-NOT transformation with larger fidelity than the optimal one given by $n = l \times m$ in Eq. (2.8). Thus the assumption is false and we have proven that the transposition on the 2-dimensional Hilbert space is not probabilistically realisable from finite clones of the uncorrelated input states.

The impossibility of 2-dimensional transposition implies that for larger dimensions. If the transposition on $d(\geq 3)$-dimensional Hilbert space is probabilistically realisable from finite clones, we can encode the states from $\mathbb{C}_2$ in a 2-dimensional subspace of the d-dimensional space to probabilistically realise the transposition on the 2-dimensional space. Thus the transposition on any dimensional space requires infinite clones.

The no-go theorem for state transposition presented in this section is used to prove another no-go theorem in Sec. 4.1. There we will analyse the channel transposition $\Gamma \mapsto \mathrm{T}\circ\Gamma\circ\mathrm{T}$, which can be reduced to the state transposition.

Remark 7. The applicability of our proof is not restricted to the transposition. Assume that the optimal fidelity for approximating an unphysical map $|\psi\rangle \mapsto |\psi'\rangle$ scales as

$$1-\frac{1}{f(n)}, \tag{3.11}$$

where n is the number of clones available and $f(n)$ increases monotonically according to n. If $f(n)$ grows less rapidly than $O(\exp(n))$, a similar argument to our proof for transposition reveals that the unphysical map $|\psi\rangle \mapsto |\psi'\rangle$ is not probabilistically realisable from finite clones of the input states uncorrelated to other systems.

3.2 An alternative proof

Here we give an alternative proof of the necessity of infinite clones for the transposition on the $d(\geq 3)$-dimensional space. Unlike the one presented in the previous section, the alternative proof does not refer to the preceding result on the universal-NOT transformation. Although the alternative proof does not apply to the 2-dimensional transposition, it proves no-go theorems for other kinds of positive maps.

The first lemma reveals that a positive TP map is probabilistically realisable without clones of input states if and only if it is CP, even when the input states are uncorrelated to other systems.

Lemma 8. Let $\mathcal{F}:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$ be a positive TP map. If there exists a CP map $\mathcal{E}:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$ implementing $\mathcal{F}$ probabilistically, i.e. if $\mathcal{E}$ satisfies

$$\epsilon \leq \mathrm{Tr}[\mathcal{E}(\rho)], \qquad \mathcal{E}(\rho)=\mathrm{Tr}[\mathcal{E}(\rho)]\mathcal{F}(\rho) \qquad (\forall\rho\in\mathcal{S}(\mathcal{H})), \tag{3.12}$$

for some positive real number $\epsilon > 0$, then either $\mathcal{F}(\cdot) = \rho\mathrm{Tr}[\cdot]$ or $\mathcal{F} = \mathcal{E}/p$ with some positive number p. In particular, $\mathcal{F}$ is CP in this case.

Proof. We consider the action of $\mathcal{E}$ on a probabilistic mixture $p\rho + (1-p)\sigma$ of two states ρ and σ in $\mathcal{S}(\mathcal{H})$. By the assumption Eq. (3.12),

$$\begin{aligned}\mathcal{E}(p\rho + (1-p)\sigma) &= \mathrm{Tr}[\mathcal{E}(p\rho + (1-p)\sigma)]\mathcal{F}(p\rho + (1-p)\sigma) \\ &= \mathrm{Tr}[\mathcal{E}(\sigma)]\mathcal{F}(\sigma) + p\{\mathrm{Tr}[\mathcal{E}(\sigma)]\mathcal{F}(\rho-\sigma) + \mathrm{Tr}[\mathcal{E}(\rho-\sigma)]\mathcal{F}(\sigma)\} \\ &\quad + p^2\mathrm{Tr}[\mathcal{E}(\rho-\sigma)]\mathcal{F}(\rho-\sigma). \end{aligned} \tag{3.13}$$

On the other hand, the linearity of $\mathcal{E}$ implies

$$\begin{aligned}\mathcal{E}(p\rho + (1-p)\sigma) &= p\mathcal{E}(\rho) + (1-p)\mathcal{E}(\sigma) \\ &= p\mathrm{Tr}[\mathcal{E}(\rho)]\mathcal{F}(\rho) + (1-p)\mathrm{Tr}[\mathcal{E}(\sigma)]\mathcal{F}(\sigma) \\ &= \mathrm{Tr}[\mathcal{E}(\sigma)]\mathcal{F}(\sigma) + p\{\mathrm{Tr}[\mathcal{E}(\rho)]\mathcal{F}(\rho) - \mathrm{Tr}[\mathcal{E}(\sigma)]\mathcal{F}(\sigma)\}. \end{aligned} \tag{3.14}$$

Since Eq. (3.13)= Eq. (3.14) must hold for all p, in particular, the third term in Eq. (3.13) must be zero:

$$\mathrm{Tr}[\mathcal{E}(\rho-\sigma)]\mathcal{F}(\rho-\sigma) = 0. \tag{3.15}$$

If $\mathcal{F}$ returns a fixed output state for any input state, then the statement of the lemma holds trivially.

Otherwise if there are states $\rho,\ \sigma \in \mathcal{S}(\mathcal{H})$ satisfying $\mathcal{F}(\rho) \neq \mathcal{F}(\sigma)$, then for any state $\tau \in \mathcal{S}(\mathcal{H})$, $\mathcal{F}(\rho) \neq \mathcal{F}(\tau)$ or $\mathcal{F}(\sigma) \neq \mathcal{F}(\tau)$ hold. In both cases, Eq. (3.15) implies $\mathrm{Tr}[\mathcal{E}(\rho)] = \mathrm{Tr}[\mathcal{E}(\sigma)] = \mathrm{Tr}[\mathcal{E}(\tau)]$. Thus if there are states $\rho,\ \sigma \in \mathcal{S}(\mathcal{H})$ satisfying $\mathcal{F}(\rho) \neq \mathcal{F}(\sigma)$, there is a constant $p \in (0, 1])$ such that

$$p = \mathrm{Tr}[\mathcal{E}(\tau)] \qquad (\forall \tau \in \mathcal{S}(\mathcal{H})), \tag{3.16}$$

which implies $\mathcal{F} = \mathcal{E}/p$. □

The following lemma reveals that a certain kind of positive maps are not probabilistically realisable from finite clones of the unknown input states uncorrelated to other systems.

Lemma 9. Let $\mathcal{H}$ be a Hilbert space and $\mathcal{F} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ be a positive TP map. If there is a subspace $\mathcal{H}' \subsetneq \mathcal{H}$ (whose orthogonal complement denoted by $\mathcal{H}'^{\perp}$) such that

- the restriction of $\mathcal{F}$ to $\mathcal{H}'$, denoted by $\mathcal{F}' : \mathcal{B}(\mathcal{H}') \to \mathcal{B}(\mathcal{K})$ is not CP, and
- there exists a subspace $\mathcal{K}' \subsetneq \mathcal{K}$ such that the ranges of $\mathcal{F}' : \mathcal{B}(\mathcal{H}') \to \mathcal{B}(\mathcal{K})$ and the restriction of $\mathcal{F}$ to $\mathcal{H}'^{\perp}$, denoted by $\mathcal{F}'_{\perp} : \mathcal{B}(\mathcal{H}'^{\perp}) \to \mathcal{B}(\mathcal{K})$, are included in $\mathcal{B}(\mathcal{K}')$ and $\mathcal{B}(\mathcal{K}'^{\perp})$, respectively,

then there is no positive integer n and CP map $\mathcal{E} : \mathcal{B}(\mathcal{H}^{\otimes n}) \to \mathcal{B}(\mathcal{K})$ satisfying

$$\epsilon \leq \mathcal{E}(\rho^{\otimes n}) \propto \mathcal{F}(\rho) \qquad (\forall \rho \in \mathcal{S}(\mathcal{H})), \tag{3.17}$$

for some positive real number ϵ.

Proof. Let us assume that such $\mathcal{E}$ exists. We can symmetrise $\mathcal{E}$ with regard to permutations of n input systems by $\mathcal{E}' = (n!)^{-1} \sum_{\text{SWAP:swap operation of } n \text{ systems}} \mathcal{E} \circ$ SWAP. The resulting map $\mathcal{E}'$ also satisfies the assumption (3.17). From now on, we assume that $\mathcal{E}$ is already symmetrised.

We consider the action of $\mathcal{E}$ on n-clones of a probabilistic mixture $p\rho + (1-p)\sigma$ of two states $\rho,\ \sigma \in \mathcal{S}(\mathcal{H})$. By the assumption (3.17), linearity, and permutation symmetry of $\mathcal{E}$,

$$\begin{aligned}
& \mathcal{E}((p\rho + (1-p)\sigma)^{\otimes n}) \\
= \ & \mathrm{Tr}[\mathcal{E}((p\rho + (1-p)\sigma)^{\otimes n})]\mathcal{F}(p\rho + (1-p)\sigma) \\
= \ & \left\{ \sum_{k=0}^{n} p^k \binom{n}{k} \mathrm{Tr}[\mathcal{E}(\sigma^{\otimes n-k} \otimes (\rho - \sigma)^{\otimes k})] \right\} \times \left\{ \mathcal{F}(\sigma) + p\mathcal{F}(\rho - \sigma) \right\}, \\
= \ & \sum_{k=0}^{n+1} p^k \left\{ \binom{n}{k} \mathrm{Tr}[\mathcal{E}(\sigma^{\otimes n-k} \otimes (\rho - \sigma)^{\otimes k})]\mathcal{F}(\sigma) \right. \\
& \left. + \binom{n}{k-1} \mathrm{Tr}[\mathcal{E}(\sigma^{\otimes n-k+1} \otimes (\rho - \sigma)^{\otimes k-1})]\mathcal{F}(\rho - \sigma) \right\} \qquad (3.18)
\end{aligned}$$

where we adopt the convention $\binom{n}{n+1} = \binom{n}{-1} = 0$. On the other hand $\mathcal{E}((p\rho + (1-p)\sigma)^{\otimes n})$ is also expanded as

$$\begin{aligned}
\mathcal{E}((p\rho + (1-p)\sigma)^{\otimes n}) &= \mathcal{E}((\sigma + p(\rho - \sigma))^{\otimes n}) \\
&= \sum_{k=0}^{n} p^k \binom{n}{k} \mathcal{E}(\sigma^{\otimes n-k} \otimes (\rho - \sigma)^{\otimes k}). \qquad (3.19)
\end{aligned}$$

Since Eq. (3.18)=Eq. (3.19) holds for all $p \in (0, 1]$, p^k's matrix coefficients in Eq. (3.18) and Eq. (3.19) must be equal for each k. In particular the equation for $k = 1$ leads

$$\mathcal{E}(\sigma^{\otimes n-1} \otimes (\rho - \sigma)) = \mathrm{Tr}[\mathcal{E}(\sigma^{\otimes n-1} \otimes (\rho - \sigma))]\mathcal{F}(\sigma) + \frac{\mathrm{Tr}[\sigma^{\otimes n}]}{n}\mathcal{F}(\rho - \sigma).$$

This equation is simplified to

$$\mathcal{E}(\sigma^{\otimes n-1} \otimes \rho) = \frac{\mathrm{Tr}[\mathcal{E}(\sigma^{\otimes n})]}{n}\mathcal{F}(\rho) + \frac{\mathrm{Tr}[\mathcal{E}(\sigma^{\otimes n-1} \otimes (n\rho - \sigma))]}{n}\mathcal{F}(\sigma), \qquad (3.20)$$

by using the assumption (3.17).

Let us take ρ and σ from the spaces $\mathcal{S}(\mathcal{H}')$ and $\mathcal{S}(\mathcal{H}'^{\perp})$, respectively. From Eq. (3.20) and the second condition of $\mathcal{F}$, the CP map $\mathcal{U}[\Pi_{\mathcal{K}'}] \circ \mathcal{E}$ satisfies

$$\mathcal{U}[\Pi_{\mathcal{K}'}] \circ \mathcal{E}(\sigma^{\otimes n-1} \otimes \rho) = \frac{\mathrm{Tr}[\mathcal{E}(\sigma^{\otimes n})]}{n}\mathcal{F}'(\rho). \qquad (3.21)$$

The map $\mathcal{U}[\Pi_{\mathcal{K}'}] \circ \mathcal{E}(\sigma^{\otimes n-1} \otimes \cdot) : \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{K}_1)$ probabilistically realises non-CP map $\mathcal{F}'$ without cloned input states. This contradicts to Lem. 8, and thus the existence assumption of $\mathcal{E}$ is false. □

Transpositions on $d(\geq 3)$-dimensional Hilbert spaces satisfy the two conditions in Lem. 9. If $\{|i\rangle\}_{i=1,...,d}$ is the basis of the transposition, take subspaces $\mathcal{H}' = \mathrm{span}\{|i\rangle \mid i = 1, ..., d-1\}$ and $\mathcal{H}'^{\perp} = \mathrm{span}\{|d\rangle\}$. Then $\mathcal{F}'$ is the transposition on $d-1$-dimensional subspace. Another class of positive maps satisfying the conditions of Lem. 9 is that decomposes to

$$\mathcal{F} = \mathcal{F}' \circ \mathcal{U}[\Pi_{\mathcal{H}'}] + \mathcal{F}'_{\perp} \circ \mathcal{U}[\Pi_{\mathcal{H}'^{\perp}}], \tag{3.22}$$

with projectors $\Pi_{\mathcal{H}'}$ and $\Pi_{\mathcal{H}'^{\perp}}$, positive non-CP map $\mathcal{F}' : \mathcal{B}(\mathcal{H}') \to \mathcal{B}(\mathcal{K}')$, and positive map $\mathcal{F}'_{\perp} : \mathcal{B}(\mathcal{H}'^{\perp}) \to \mathcal{B}(\mathcal{K}'^{\perp})$.

Consider following hypothesis: if a TP positive non-CP map $\mathcal{F}' : \mathcal{B}(\mathcal{H}') \to \mathcal{B}(\mathcal{K}')$ is probabilistically realisable from finite clones, then the positive non-CP map $\mathcal{F} : \mathcal{B}(\mathcal{H}' \oplus \mathbb{C}) \to \mathcal{B}(\mathcal{K}' \oplus \mathbb{C})$ defined by

$$\mathcal{F} := \mathcal{F}' \circ \mathcal{U}[\Pi_{\mathcal{H}'}] + \mathrm{id}_{\mathbb{C}} \circ \mathcal{U}[\Pi_{\mathbb{C}}], \tag{3.23}$$

is also probabilistically realisable from finite clones. If this hypothesis is true then Lem. 9 implies the non-realisability of any positive non-CP maps. We neither prove or disprove this hypothesis. No matter if this hypothesis is false or true, we conjecture that every positive TP non-CP map is not probabilistically realisable from finite clones. In other words, we conjecture that the gap between positive and CP maps in terms of probabilistic realisability, is not filled by adding finite power of non-linearity to quantum theory.

Chapter 4

Transposition on channels

Here we shift our target from maps to supermaps. As we have seen in Sec. 2.2.1, the channel transposition $\Gamma \mapsto \mathrm{T} \circ \Gamma \circ \mathrm{T}$ is a positive non-CP supermap, and thus is not deterministically realisable without replicas of the input TPCP map. We relax the linearity constraint from quantum theory by allowing replicas of input TPCP maps, in a similar way we have done with state clones in Chap. 3. Any nonlinear supermaps on uncorrelated maps becomes realisable if infinite replicas of the input TPCP maps is available, and the gap between positive and CP maps closes. In this chapter, we investigate the behaviour of this gap in quantum theory with limited non-linearity, by analysing the probabilistic realisability of channel transposition with replicas.

As mentioned in the introduction, supermaps sometimes behave differently from maps. It turns out that if the unknown TPCP map Γ is a unitary channel $\mathcal{U}[U]$, the *unitary conjugation* $\mathcal{U}[U] \mapsto \mathrm{T} \circ \mathcal{U}[U] \circ \mathrm{T} = \mathcal{U}[U^*]$ is realisable from *finite* number of replicas of $\mathcal{U}[U]$, despite infinite clones are required for state transposition (see Chap. 3). We analyse this fact deeply and relate it with a particle-hole exchange channel in fermionic systems. Our analysis on unitary conjugation is also applicable to the computation of conjugation induced quantities of entanglement.

It is shown that probabilistic channel transposition is impossible for general TPCP maps in Sec. 4.1. Section 4.2 is devoted to unitary conjugation with and without replication. Finally we propose a method to construct observables for the conjugation induced quantities in Sec. 4.3.

4.1 General channel transposition

We here briefly comment that *channel transposition* is not probabilistically realisable from finite replicas even when the input TPCP maps is not correlated to other system in their Choi operator representation (see Sec. 1.2.2 for details), and when we can use the TPCP maps sequentially[1]. Some readers may notice this just by looking Fig. 4.1. To see this fact concretely, we denote the replicated TPCP maps $\Gamma : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ by specifying the input and output spaces ex-

[1]We assume the dimension of TPCP map's output to be greater than 1, since otherwise the TPCP map is equivalent to the tracing operation Tr which does not change under transposition $\mathrm{Tr} = \mathrm{Tr} \circ \mathrm{T}$.

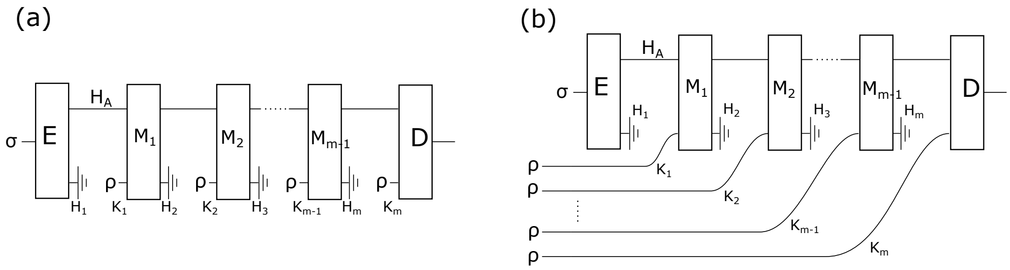

Figure 4.1: (a) The quantum circuit representations of the composition of maps presented by Eq. (4.2). The TPCP maps $\Gamma^\rho(\cdot) = \rho\ \mathrm{Tr}[\cdot]$ for generating states ρ are inserted as oracles. (b) The quantum circuit representations of the composition of maps presented by Eq. (4.3). It is clear that the output state of (b) is equals to that of (a) since the quantum circuit (b) is obtained just by extending wires of (a). The extended wires are represented by identity maps inserted in Eq. (4.3).

plicitly $\Gamma_i : \mathcal{B}(\mathcal{H}_i) \to \mathcal{B}(\mathcal{K}_i)$ $(i = 1, ..., m)$, so that the CP maps $\mathcal{E}$, $\mathcal{D}$, and $\mathcal{M}_i$ appearing in Eq. (1.14) have domains and codomains $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_1)$, $\mathcal{D} : \mathcal{B}(\mathcal{H}_A \otimes \mathcal{K}_m) \to \mathcal{B}(\mathcal{K})$, and $\mathcal{M}_i : \mathcal{B}(\mathcal{H}_A \otimes \mathcal{K}_i) \to \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_{i+1})$ (see Fig. 4.1 for clarifying these labellings).

Lemma 10. If $\dim \mathcal{K} \geq 2$, the channel transposition is not probabilistically realisable from finite replicas of uncorrelated TPCP maps. There is no TNICP maps $\mathcal{E}$, $\mathcal{D}$, and $\mathcal{M}_i$ such that

$$\begin{aligned}
&\mathcal{D} \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \Gamma_m) \circ \mathcal{M}_{m-1} \circ ... \circ \mathcal{M}_1 \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \Gamma_1) \circ \mathcal{E}(\sigma) \propto \mathrm{T} \circ \Gamma \circ \mathrm{T}(\sigma), \\
&0 < \epsilon \leq \mathrm{Tr}[\mathcal{D} \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \Gamma_m) \circ \mathcal{M}_{m-1} \circ ... \circ \mathcal{M}_1 \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \Gamma_1) \circ \mathcal{E}(\sigma)], \\
&\qquad (\forall \rho \in \mathcal{S}(\mathcal{H}),\ \forall \text{TPCP map } \Gamma : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K}))
\end{aligned}$$

for some positive number ϵ.

Proof. For any state $\rho \in \mathcal{S}(\mathcal{K})$ there is a TPCP map $\Gamma^\rho : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ producing ρ regardless of the input state. Explicitly, Γ^ρ is defined by

$$\Gamma^\rho(a) = \mathrm{Tr}[a]\rho \qquad (\forall a \in \mathcal{B}(\mathcal{H})), \tag{4.1}$$

and its transposition $\mathrm{T} \circ \Gamma^\rho \circ \mathrm{T}$ is $\Gamma^{\rho^{\mathrm{T}}}$. If the channel transposition is probabilistically realisable from finite, say, m-replicas by using the CP maps $\mathcal{E}$, $\mathcal{D}$ and $\mathcal{M}_i$, then by inserting $\Gamma = \Gamma^\rho$ to Eq. (1.14), we obtain

$$\begin{aligned}
\rho^{\mathrm{T}} &= \Gamma^{\rho^{\mathrm{T}}}(\sigma) \\
&\propto \mathcal{D}(\cdot \otimes \rho_{\mathcal{K}_m}) \circ \mathrm{Tr}_{\mathcal{H}_m} \circ \mathcal{M}_{m-1} \circ ... \circ \mathcal{M}_2(\cdot \otimes \rho_{\mathcal{K}_2}) \\
&\quad \circ \mathrm{Tr}_{\mathcal{H}_2} \circ \mathcal{M}_1(\cdot \otimes \rho_{\mathcal{K}_1}) \circ \mathrm{Tr}_{\mathcal{H}_1} \circ \mathcal{E}(\sigma), \qquad (4.2) \\
&= \mathcal{D} \circ (\mathrm{Tr}_{\mathcal{H}_m} \circ \mathcal{M}_{m-1} \otimes \mathrm{id}_{\mathcal{K}_m}) \circ ... \circ (\mathrm{Tr}_{\mathcal{H}_2} \circ \mathcal{M}_1 \otimes \mathrm{id}_{\otimes_{2=1}^m \mathcal{K}_i}) \\
&\quad \circ (\mathrm{Tr}_{\mathcal{H}_1} \circ \mathcal{E} \otimes \mathrm{id}_{\otimes_{i=1}^m \mathcal{K}_i})(\sigma \otimes_{i=1}^m \rho_{\mathcal{K}_i}). \qquad (4.3)
\end{aligned}$$

for any $\sigma \in \mathcal{S}(\mathcal{H})$. The transformation from Eq. (4.2) to Eq. (4.3) is represented by quantum circuits in Fig. 4.1. Equation (4.3) implies that a CP map from $\mathcal{B}(\otimes_{i=1}^m \mathcal{K}_i)$ to $\mathcal{B}(\mathcal{H})$ defined by the composition

$$\mathcal{D} \circ (\mathrm{Tr}_{\mathcal{H}_m} \circ \mathcal{M}_{m-1} \otimes \mathrm{id}_{\mathcal{K}_m}) \circ ... \circ (\mathrm{Tr}_{\mathcal{H}_1} \circ \mathcal{E} \otimes \mathrm{id}_{\otimes_{i=1}^m \mathcal{K}_i})(\sigma \otimes \cdot)$$

realises state transposition from m-clones, which contradicts the no-go results of state transposition presented in Sec. 3.1. $\square$

4.2 Unitary conjugation

Although general channel transposition turned out impossible from finite replicas, there is a possibility to realise the transposition on restricted sets of TPCP maps. In this section, we focus on the realisability of unitary conjugation, which is equivalent to the channel transposition on unitary channels. Note that unitaries are inevitably uncorrelated to other systems since their corresponding Choi operator representations are pure.

In Sec. 4.2.1 we show that the unitary conjugation is not probabilistically realisable without replicated unitaries if $\dim \mathcal{H} \geq 3$. In contrast, we show in Sec. 4.2.2 that deterministic unitary conjugation is possible from finite replicas of unitaries. The scheme to realise this is understood from a relation between particles and holes in Sec. 4.2.3.

4.2.1 Unitary conjugation without replicas

Let us consider unitary conjugation of untiaries on $\mathcal{H}$, where $\dim \mathcal{H}$ is denoted by d. The fact that unitary conjugation being realisable when $d = 2$ already reveals a difference between unitary conjugation and channel transposition, since we have already shown that the latter is impossible even with finite replicas. This fact motivates us to investigate realisability of unitary conjugation when $d \geq 3$. In this subsection, we consider probabilistic realisability without replication.

The optimal fidelity (2.22) for approximate unitary conjugation being less than 1 when $d \geq 3$ implies that unitary conjugation is not deterministically realisable without replication when $d \geq 3$, although it does not deny the probabilistic realisability. We however obtained a no-go theorem presented below. In spite of the lengthy proof, we do not leave it to appendix since it leads to a method to compute conjugate induced quantities presented in Sec. 4.3.

Theorem 11. [84] A unitary conjugation for d-dimensional unitaries with d greater than 2 is not probabilistically realisable without replicas. When $\mathcal{H}$ is a $d \geq 3$ dimensional Hilbert space, there is no pair of TNICP maps $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H} \otimes \mathcal{H}_A)$ and $\mathcal{D} : \mathcal{B}(\mathcal{H} \otimes \mathcal{H}_A) \to \mathcal{B}(\mathcal{H})$ such that

$$0 < \epsilon \leq \mathrm{Tr}[\mathcal{D} \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \mathcal{U}[U]) \circ \mathcal{E}(\rho)], \tag{4.4}$$

$$\mathcal{D} \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \mathcal{U}[U]) \circ \mathcal{E}(\rho) \propto \mathcal{U}[U^*](\rho), \tag{4.5}$$

$$(\forall \rho \in \mathcal{S}(\mathcal{H}))$$

for any unitary U on $\mathcal{H}$, for some positive number ϵ.

Proof. Assume that a pair of such TNICP maps $\mathcal{E}$ and $\mathcal{D}$ exists. For later use we label the domain and codomain Hilbert spaces $\mathcal{H}$ of $\mathcal{E}$ and $\mathcal{D}$ differently so that

$$\mathcal{E} : \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_A), \qquad \mathcal{D} : \mathcal{B}(\mathcal{K}_1 \otimes \mathcal{H}_A) \to \mathcal{K}_2. \tag{4.6}$$

These Hilbert spaces except $\mathcal{H}_A$ are all equivalent $\mathcal{H}_1 \cong \mathcal{H}_2 \cong \mathcal{K}_1 \cong \mathcal{K}_2$.

Assumptions (4.4) and (4.5) together imply

$$\mathcal{D} \circ (\mathrm{id}_{\mathcal{H}_A} \otimes \mathcal{U}[U]) \circ \mathcal{E} \propto \mathcal{U}[U^*], \tag{4.7}$$

which is apparently stronger than (4.5). This is because Lem. 8 tells us that either (4.7) or $\mathcal{U}[U](\cdot) = \sigma \mathrm{Tr}[\cdot]$ holds under these assumptions. Obviously the latter is not the case.

From Lem. 2 there is a CP map $\mathscr{S} : \mathrm{Pos}(\mathcal{H}_1 \otimes \mathcal{K}_1) \to \mathrm{Pos}(\mathcal{H}_2 \otimes \mathcal{K}_2)$ such that the supermap $f_{\mathscr{S}}$ defined by $\mathscr{S}$ via Eq. (1.17) is equivalent to a probabilistic unitary conjugation. Equations (4.7) and (1.18) imply $f_{\mathscr{S}}(\mathcal{U}[U]) \propto \mathcal{U}[U^*]$ for any unitary U on $\mathcal{H}$. This condition on $f_{\mathscr{S}}$ is rewritten in terms of $\mathscr{S}$ as

$$\mathscr{S}(\mathrm{id}_{\mathcal{H}_1} \otimes \mathcal{U}[U](\Phi_{\mathcal{H}_1 \otimes \mathcal{H}_1})) \propto \mathrm{id}_{\mathcal{H}_2} \otimes \mathcal{U}[U^*](\Phi_{\mathcal{H}_2 \otimes \mathcal{H}_2}) \ (\forall U), \tag{4.8}$$

where $\Phi_{\mathcal{H},\mathcal{H}}$ represents the unnormalised density operator for vector $\sum_{i=1}^{d} |i, i\rangle$, and domains and codomains of unitary operators are considered to be $U : \mathcal{H}_1 \to \mathcal{K}_1$ and $U : \mathcal{H}_2 \to \mathcal{K}_2$. In short, $\mathrm{id}_{\mathcal{H}_1} \otimes \mathcal{U}[U](\Phi_{\mathcal{H}_1 \otimes \mathcal{H}_1})$ is the Choi operator of unitary channel $\mathcal{U}[U]$.

From $\mathscr{S}$, we construct another CP map $\mathscr{S}' : \mathrm{Pos}(\mathcal{H}_1 \otimes \mathcal{K}_1) \to \mathrm{Pos}(\mathcal{H}_2 \otimes \mathcal{K}_2)$ satisfying

$$\mathcal{U}[V_{\mathcal{H}_2} \otimes W_{\mathcal{K}_2}] \circ \mathscr{S}' \circ \mathcal{U}[V_{\mathcal{H}_1}^{\mathrm{T}} \otimes W_{\mathcal{K}_1}^{\mathrm{T}}] = \mathscr{S}' \tag{4.9}$$

for all d-dimensional unitary operators V and W whose space is indicated by the subscripts. Let us consider applying $\mathscr{S}$ on the Choi operator of a sequence of unitaries $V^{\mathrm{T}} U W$. On the one hand, we obtain

$$\begin{aligned} & \mathscr{S}\left(\mathcal{U}[\mathbb{I}_{\mathcal{H}_1} \otimes V_{\mathcal{K}_1}^{\mathrm{T}} U W_{\mathcal{H}_1}](\Phi_{\mathcal{H}_1,\mathcal{H}_1})\right) \\ = \ & \mathscr{S}\left(\mathcal{U}[W_{\mathcal{H}_1}^{\mathrm{T}} \otimes V_{\mathcal{K}_1}^{\mathrm{T}} U](\Phi_{\mathcal{H}_1,\mathcal{H}_1})\right) \\ = \ & \mathscr{S} \circ \mathcal{U}[W_{\mathcal{H}_1}^{\mathrm{T}} \otimes V_{\mathcal{K}_1}^{\mathrm{T}}] \left(\mathcal{U}[\mathbb{I}_{\mathcal{H}_1} \otimes U](\Phi_{\mathcal{H}_1,\mathcal{H}_1})\right), \end{aligned} \tag{4.10}$$

where we have used the relation

$$\mathbb{I} \otimes X \sum_{i=1}^{d} |i, i\rangle = X^{\mathrm{T}} \otimes \mathbb{I} \sum_{i=1}^{d} |i, i\rangle \tag{4.11}$$

satisfied for any operator X on $\mathcal{H}$. On the other hand, the defining property of $\mathscr{S}$ given by Eq. (4.8) together with the relation (4.11) implies

$$\begin{aligned} & \mathscr{S}\left(\mathcal{U}[\mathbb{I}_{\mathcal{H}_1} \otimes V_{\mathcal{K}_1}^{\mathrm{T}} U W_{\mathcal{H}_1}](\Phi_{\mathcal{H}_1,\mathcal{H}_1})\right) \\ \propto \ & \mathcal{U}[\mathbb{I}_{\mathcal{H}_2} \otimes V_{\mathcal{K}_2}^{\dagger} U^* W_{\mathcal{H}_2}^{*}](\Phi_{\mathcal{H}_2,\mathcal{H}_2}) \\ = \ & \mathcal{U}[W_{\mathcal{H}_2}^{\dagger} \otimes V_{\mathcal{K}_2}^{\dagger} U^*](\Phi_{\mathcal{H}_2,\mathcal{H}_2}) \\ = \ & \mathcal{U}[W_{\mathcal{H}_2}^{\dagger} \otimes V_{\mathcal{K}_2}^{\dagger}] \left(\mathcal{U}[\mathbb{I}_{\mathcal{H}_2} \otimes U^*](\Phi_{\mathcal{H}_2,\mathcal{H}_2})\right). \end{aligned} \tag{4.12}$$

By equating (4.10) and (4.12), we obtain

$$\mathcal{U}[W_{\mathcal{H}_2} \otimes V_{\mathcal{K}_2}] \circ \mathscr{S} \circ \mathcal{U}[W_{\mathcal{H}_1}^{\mathrm{T}} \otimes V_{\mathcal{K}_1}^{\mathrm{T}}] \left(\mathcal{U}[\mathbb{I}_{\mathcal{H}_1} \otimes U](\Phi_{\mathcal{H}_1,\mathcal{H}_1})\right) \propto \mathcal{U}[\mathbb{I}_{\mathcal{H}_2} \otimes U^*](\Phi_{\mathcal{H}_2,\mathcal{H}_2}).$$

This implies that the CP map $\mathscr{S}_{V,W}$ defined by

$$\mathscr{S}_{V,W} := \mathcal{U}[W_{\mathcal{H}_2} \otimes V_{\mathcal{K}_2}] \circ \mathscr{S} \circ \mathcal{U}[W_{\mathcal{H}_1}^{\mathrm{T}} \otimes V_{\mathcal{K}_1}^{\mathrm{T}}],$$

satisfies Eq. (4.8) and thus represents a CP map for unitary conjugation. We define the CP map $\mathscr{S}'$ by

$$\mathscr{S}' := \int dV dW \mathscr{S}_{V,W}, \tag{4.13}$$

where integral is taken by the normalised SU(d) Haar measure[2]. The symmetry (4.9) is guaranteed by construction. From now on, we assume that $\mathscr{S}$ already satisfies Eq. (4.9).

For further analysis it is convenient to represent the symmetry constraint (4.9) in terms of $\mathscr{S}$'s Choi matrix. Let $\widetilde{\mathscr{S}} \in \mathrm{Pos}(\otimes_{i=1}^{2}\mathcal{H}_i \otimes \mathcal{K}_i)$ be a Choi matrix of $\mathscr{S}$ defined by

$$\widetilde{\mathscr{S}} = \mathrm{id}_{\mathcal{H}_1\otimes\mathcal{K}_1} \otimes \mathscr{S}(\Phi_{\mathcal{H}_1,\mathcal{H}_1} \otimes \Phi_{\mathcal{K}_1,\mathcal{K}_1}). \tag{4.14}$$

Then the symmetry constraint (4.9) is equivalent to

$$\widetilde{\mathscr{S}} = \mathcal{U}[V_{\mathcal{H}_1} \otimes V_{\mathcal{H}_2} \otimes W_{\mathcal{K}_1} \otimes W_{\mathcal{K}_2}](\widetilde{\mathscr{S}}), \tag{4.15}$$

for all $V,\ W \in \mathrm{SU}(d)$ (see Rem. 12 for detail). If the operator Schmidt decomposition of $\widetilde{\mathscr{S}}$ with regard to the subsystems $\mathcal{B}(\mathcal{H}_1\otimes\mathcal{H}_2)$ and $\mathcal{B}(\mathcal{K}_2\otimes\mathcal{K}_2)$ (see Appx. A for the definition of the operator Schmidt decomposition) is

$$\widetilde{\mathscr{S}} = \sum_k \gamma_k^{enc} \otimes \gamma_k^{dec}, \tag{4.16}$$

each operator $\gamma_k^{enc} \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ and $\gamma_k^{dec} \in \mathcal{B}(\mathcal{K}_1 \otimes \mathcal{K}_2)$ must satisfy

$$\gamma_k^{enc} = \mathcal{U}[V_{\mathcal{H}_1} \otimes V_{\mathcal{H}_2}](\gamma_k^{enc}), \qquad \gamma_k^{dec} = \mathcal{U}[W_{\mathcal{K}_1} \otimes W_{\mathcal{K}_2}](\gamma_k^{dec}), \tag{4.17}$$

because of the invariance Eq. (4.15). Then Schur's lemma (see e.g. Lem. 2.7 in Ref. [85]) implies the following form for γ_k^{enc} and γ_k^{dec}:

$$\gamma_k^{enc} = a_k\Pi_{\mathrm{S}(\mathcal{H}_1\otimes\mathcal{H}_2)} + b_k\Pi_{\mathrm{A}(\mathcal{H}_1\otimes\mathcal{H}_2)},\ \gamma_k^{dec} = c_k\Pi_{\mathrm{S}(\mathcal{K}_1\otimes\mathcal{K}_2)} + d_k\Pi_{\mathrm{A}(\mathcal{K}_1\otimes\mathcal{K}_2)}, \tag{4.18}$$

where $\Pi_{\mathrm{S}(\mathcal{H}\otimes\mathcal{H})}$ and $\Pi_{\mathrm{A}(\mathcal{H}\otimes\mathcal{H})}$ are projectors onto the symmetric and antisymmetric subspaces of $\mathcal{H}\otimes\mathcal{H}$, and a_k, b_k, c_k, d_k are complex coefficients. By substituting γ's

[2]If G is a group and a measurable set at the same time, then the Haar measure μ on G is a particular measure such that $\mu(Bg) = \mu(gB) = \mu(B)$, for any measurable subset B of G and $g \in G$. Here, gB and Bg represent the measurable subsets obtained by left and right element-wise actions of g on B. The Haar measure is unique up to some constant factor. If the constant is taken so that $\mu(G) = 1$, it is called the normalised Haar measure. The normalised Haar measures exist for any compact Lie groups including U(d) and SU(d) groups. See e.g. Ref. [85] for more details.

from Eqs. (4.18) into Eq. (4.16), we obtain the following decomposition of $\widetilde{\mathscr{S}}$:

$$\begin{aligned}\widetilde{\mathscr{S}} = & \left(\sum_k a_k c_k\right) \Pi_{\mathrm{S}(\mathcal{H}_1\otimes\mathcal{H}_2)} \otimes \Pi_{\mathrm{S}(\mathcal{K}_1\otimes\mathcal{K}_2)} + \left(\sum_k a_k d_k\right) \Pi_{\mathrm{S}(\mathcal{H}_1\otimes\mathcal{H}_2)} \otimes \Pi_{\mathrm{A}(\mathcal{K}_1\otimes\mathcal{K}_2)} \\ + & \left(\sum_k b_k c_k\right) \Pi_{\mathrm{A}(\mathcal{H}_1\otimes\mathcal{H}_2)} \otimes \Pi_{\mathrm{S}(\mathcal{K}_1\otimes\mathcal{K}_2)} + \left(\sum_k b_k d_k\right) \Pi_{\mathrm{A}(\mathcal{H}_1\otimes\mathcal{H}_2)} \otimes \Pi_{\mathrm{A}(\mathcal{K}_1\otimes\mathcal{K}_2)}.\end{aligned} \tag{4.19}$$

The Choi operator $\widetilde{\mathscr{S}}$ must be positive semi-definite since $\mathscr{S}$ is CP. This implies that the coefficients of Eq. (4.19) must all be non-negative, and $\widetilde{\mathscr{S}}$ is now decomposed into

$$\widetilde{\mathscr{S}} = \sum_{i,j\in\{\mathrm{S},\mathrm{A}\}} p_{ij} \Pi_{i(\mathcal{H}_1\otimes\mathcal{H}_2)} \otimes \Pi_{j(\mathcal{K}_1\otimes\mathcal{K}_2)} \tag{4.20}$$

with non-negative real numbers p_{ij}.

Now we return to $\mathscr{S}$ from the Choi operator $\widetilde{\mathscr{S}}$. Let us denote the CP maps whose Choi matrices are $\Pi_{i(\mathcal{H}\otimes\mathcal{K})}$ by $\mathcal{E}_{i(\mathcal{H},\mathcal{K})} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$. The CP map $\mathscr{S}$ is decomposed to a separable form

$$\mathscr{S} = \sum_{i,j\in\{\mathrm{S},\mathrm{A}\}} p_{ij} \mathcal{E}_{i(\mathcal{H}_1,\mathcal{H}_2)} \otimes \mathcal{E}_{j(\mathcal{K}_1,\mathcal{K}_2)}. \tag{4.21}$$

Each component $\mathcal{E}_{i(\mathcal{H}_1,\mathcal{H}_2)} \otimes \mathcal{E}_{j(\mathcal{K}_1,\mathcal{K}_2)}$ must send (unnormalised) maximally entangled vectors to (unnormalised) maximally entangled vectors so that $\mathscr{S}$ satisfies Eq. (4.8). This implies that $\mathcal{E}_{i(\mathcal{H}_1,\mathcal{H}_2)} \otimes \mathrm{id}_{\mathcal{K}_1}$ and $\mathrm{id}_{\mathcal{H}_1} \otimes \mathcal{E}_{j(\mathcal{K}_1,\mathcal{K}_2)}$ both send maximally entangled states to another maximally entangled state. Equivalently, Choi matrices $\Pi_{i(\mathcal{H}_1\otimes\mathcal{H}_2)}$ and $\Pi_{j(\mathcal{K}_1\otimes\mathcal{K}_2)}$ of $\mathcal{E}_{i(\mathcal{H}_1,\mathcal{H}_2)}$ and $\mathcal{E}_{j(\mathcal{K}_1,\mathcal{K}_2)}$ must be maximally entangled states. This is impossible if $d \geq 3$ because the rank of $\Pi_{\mathrm{S}(\mathcal{H}\otimes\mathcal{K})}$ and $\Pi_{\mathrm{A}(\mathcal{H}\otimes\mathcal{K})}$ are the dimensions of symmetric and antisymmetric subspaces given by $d(d+1)/2$ and $d(d-1)/2$, respectively. Thus there is no CP map $\mathscr{S}$ representing a probabilistic unitary conjugation without replicas if $d \geq 3$. □

Outlining the proof, an admissible 2-map $\mathscr{S}$ is first reduced to a canonical form with symmetry (4.9) by the assumption that $\mathscr{S}$ represents unitary conjugation. Then $\mathscr{S}$'s symmetry (4.9) is translated to (4.15) for $\mathscr{S}$'s Choi operator $\widetilde{\mathscr{S}}$. Simple group theory is applied for disproving the existence of Choi operator $\widetilde{\mathscr{S}}$ with this symmetry.

This proof does not apply to the case $d = 2$, since the antisymmetric subspace of $\mathcal{H} \otimes \mathcal{H}$ has dimension $d(d-1)/2 = 1$. Antisymmetric subspaces also play an important role in the next section where we consider probabilistic realisability from finite replicas.

Remark 12. An important step in the proof is the translation of $\mathscr{S}$'s symmetry (4.9) to its Choi operator's symmetry (4.15). If a linear map $\mathscr{S} : \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{K}_1) \to \mathcal{B}(\mathcal{H}_2 \otimes \mathcal{K}_2)$ satisfies

$$\mathscr{S} = \mathcal{U}[U_{\mathcal{K}_1} \otimes V_{\mathcal{K}_2}] \circ \mathscr{S} \circ \mathcal{U}[U^{\mathrm{T}}_{\mathcal{H}_1} \otimes V^{\mathrm{T}}_{\mathcal{H}_2}], \tag{4.22}$$

then its Choi matrix satisfies

$$\begin{aligned}
\widetilde{\mathscr{S}} &:= \mathrm{id}_{\mathcal{H}_1\otimes\mathcal{K}_1} \otimes \mathscr{S}(\Phi_{\mathcal{H}_1,\mathcal{H}_1} \otimes \Phi_{\mathcal{K}_1,\mathcal{K}_1}) \\
&= \mathrm{id}_{\mathcal{H}_1\otimes\mathcal{K}_1} \otimes \left(\mathcal{U}[U_{\mathcal{K}_1} \otimes V_{\mathcal{K}_2}] \circ \mathscr{S} \circ \mathcal{U}[U_{\mathcal{H}_1}^{\mathrm{T}} \otimes V_{\mathcal{H}_2}^{\mathrm{T}}]\right) (\Phi_{\mathcal{H}_1,\mathcal{H}_1} \otimes \Phi_{\mathcal{K}_1,\mathcal{K}_1}) \\
&= \left(\mathcal{U}[U_{\mathcal{H}_1} \otimes V_{\mathcal{H}_2}] \otimes \mathcal{U}[U_{\mathcal{K}_1} \otimes V_{\mathcal{K}_2}] \circ \mathscr{S}\right) (\Phi_{\mathcal{H}_1,\mathcal{H}_1} \otimes \Phi_{\mathcal{K}_1,\mathcal{K}_1}) \\
&= \mathcal{U}[U_{\mathcal{H}_1} \otimes V_{\mathcal{H}_2} \otimes U_{\mathcal{K}_1} \otimes V_{\mathcal{K}_2}](\widetilde{\mathscr{S}}), \\
&= U_{\mathcal{H}_1} \otimes U_{\mathcal{K}_1} \otimes V_{\mathcal{H}_2} \otimes V_{\mathcal{K}_2}\, \widetilde{\mathscr{S}}\, U_{\mathcal{H}_1}^\dagger \otimes U_{\mathcal{K}_1}^\dagger \otimes V_{\mathcal{H}_2}^\dagger \otimes V_{\mathcal{K}_2}^\dagger
\end{aligned} \tag{4.23}$$

where we have used relation (4.11) in the third equality. Operators with symmetry constraint (4.23) is analysed in Refs. [80, 71] for constructing observable local unitary invariants (see Sec. 2.3.4 for details). Motivated by this fact, we propose a method to construct observables for measuring conjugation induced quantities in Sec. 4.3.

4.2.2 Unitary conjugation with replicas

We here turn to the realisability with replicas. As we have seen in Chap. 3, finitely many cloned input states are not helpful for realising state transposition. In contrast, we will see that replicas are helpful for unitary conjugation.

In the remainder of this chapter we denote the antisymmetric subspace of $\mathcal{H}^{\otimes m}$ by $\mathcal{H}^{\wedge m}$. If $\dim \mathcal{H} = d$ and $\{|i\rangle\}_{i=1,...,d}$ is a basis of $\mathcal{H}$, the antisymmetric subspace $\mathcal{H}^{\wedge m}$ is spanned by

$$|\wedge_{i_1,...,i_m}\rangle := \frac{1}{\sqrt{m}} \sum_{\tau\in \mathrm{S}_m} \mathrm{sgn}(\tau)|\tau_{i_1}, ..., \tau_{i_m}\rangle, \tag{4.24}$$

for $1 \le i_1 < ... < i_m \le d$, where S_m represents the symmetry group of order m. If we write $\tau_{i_1}, ..., \tau_{i_m}$ for $\tau \in \mathrm{S}_m$, then τ is a permutation inside $\{i_1, ..., i_m\}$, and does not exchange i_j to elements outside $\{i_1, ..., i_m\}$. The dimension of antisymmetric space is $\binom{d}{m}$.

Theorem 13. [84] If $m+n = d$, there exists a pair of TPCP maps $\mathcal{E} : \mathcal{B}(\mathcal{H}^{\otimes n}) \to \mathcal{B}(\mathcal{H}^{\otimes m})$ and $\mathcal{D} : \mathcal{B}(\mathcal{H}^{\otimes m}) \to \mathcal{B}(\mathcal{H}^{\otimes n})$, satisfying

$$\mathcal{D} \circ \mathcal{U}[U^{\otimes m}] \circ \mathcal{E}(\rho) = \mathcal{U}[U^{*\otimes n}](\rho), \tag{4.25}$$

for any unitary operator U on $\mathcal{H}$ and any state ρ on the antisymmetric subspace $\mathcal{H}^{\wedge n}$ of $\mathcal{H}^{\otimes n}$.

We construct the TPCP maps $\mathcal{E}$ and $\mathcal{D}$ satisfying Eq. (4.25). Define an operator $A_{n\to m} : \mathcal{H}^{\wedge n} \to \mathcal{H}^{\wedge m}$ by

$$A_{n\to m} := \frac{1}{\sqrt{m!n!}} \sum_{\tau\in \mathrm{S}_{n+m}} \mathrm{sgn}(\tau)|\tau_1, ..., \tau_m\rangle\langle\tau_{m+1}, ..., \tau_{m+n}|. \tag{4.26}$$

This is a unitary operator between antisymmetric subspaces $\mathcal{H}^{\wedge n}$ to $\mathcal{H}^{\wedge m}$ (see Appx. B.1 for details). When $m = n = 1$ and $d = 2$, $A_{n\to m}$ is equal to $|1\rangle\langle 2| - |2\rangle\langle 1|$, which is up-to-phase equivalent to σ_y operator. Define TPCP maps $\mathcal{E} : \mathcal{B}(\mathcal{H}^{\otimes n}) \to \mathcal{B}(\mathcal{H}^{\otimes m})$ and $\mathcal{D} : \mathcal{B}(\mathcal{H}^{\otimes m}) \to \mathcal{B}(\mathcal{H}^{\otimes n})$ by

$$\mathcal{E} = \mathcal{U}[A_{n\to m}] + \mathcal{E}', \qquad \mathcal{D} = \mathcal{U}[A^\dagger_{n\to m}] + \mathcal{D}', \tag{4.27}$$

where $\mathcal{E}' : \mathcal{B}(\mathcal{H}^{\wedge n\perp}) \to \mathcal{B}(\mathcal{H}^{\otimes m})$ and $\mathcal{D}' : \mathcal{B}(\mathcal{H}^{\wedge m\perp}) \to \mathcal{B}(\mathcal{H}^{\otimes n})$ are any TPCP maps from complement spaces of $\mathcal{H}^{\wedge n}$ and $\mathcal{H}^{\wedge m}$, respectively. These $\mathcal{E}'$ and $\mathcal{D}'$ can be anything because

$$\begin{aligned} \mathcal{D} \circ \mathcal{U}[U^{\otimes m}] \circ \mathcal{E}(\rho) &= \mathcal{D} \circ \mathcal{U}[U^{\otimes m}] \circ \mathcal{U}[A_{n\to m}](\rho) \\ &= \mathcal{U}[A^\dagger_{n\to m}] \circ \mathcal{U}[U^{\otimes m}] \circ \mathcal{U}[A_{n\to m}](\rho), \end{aligned} \tag{4.28}$$

holds for any state $\rho \in \mathcal{S}(\mathcal{H}^{\wedge n})$, no matter what $\mathcal{E}'$ and $\mathcal{D}'$ are. The right-hand-side of Eq. (4.28) is transformed by the following lemma to $\mathcal{U}[U^{*\otimes n}](\rho)$, which leads Thm. 13.

Lemma 14. [84] If $A_{n\to m}$ is the operator defined by Eq. (4.26),

$$\mathcal{U}[A_{n\to m}] \circ \mathcal{U}[U^{*\otimes n}] = \mathcal{U}[U^{\otimes m}] \circ \mathcal{U}[A_{n\to m}]. \tag{4.29}$$

holds for any unitary operator U on $\mathcal{H}$.

Proof. Note that Eq. (4.29) is rewritten into

$$\mathcal{U}[A_{n\to m}] = \mathcal{U}[U^{\otimes m}] \circ \mathcal{U}[A_{n\to m}] \circ \mathcal{U}[U^{\mathrm{T}\otimes n}]. \tag{4.30}$$

From the observation of Rem. 12, this is satisfied if and only if the Choi matrix $\widetilde{\mathcal{U}[A_{n\to m}]}$ of $\mathcal{U}[A_{n\to m}]$ satisfies $\widetilde{\mathcal{U}[A_{n\to m}]} = \mathcal{U}[U^{\otimes m+n}] \circ \widetilde{\mathcal{U}[A_{n\to m}]}$. This holds since $\widetilde{\mathcal{U}[A_{n\to m}]}$ is the projector onto the antisymmetric subspace $\mathcal{H}^{\wedge m+n}$ of $\mathcal{H}^{\otimes m+n}$ (this is almost obvious but see Appx. B.1 for details). It is invariant under the action of $\mathcal{U}[U^{\otimes m+n}]$ since the antisymmetric subspace is an irreducible subspace of $U^{\otimes m+n}$. □

Theorem 13 includes unitary conjugation as a special case.

Corollary 15. [84] Unitary conjugation of unitaries on d-dimensional Hilbert spaces is deterministically realisable from $d-1$ replicas of the unknown unitary. There is a pair of TPCP maps $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}^{\otimes d-1})$ and $\mathcal{D} : \mathcal{B}(\mathcal{H}^{\otimes d-1}) \to \mathcal{B}(\mathcal{H})$ such that $\mathcal{D} \circ \mathcal{U}[U]^{\otimes d-1} \circ \mathcal{E} = \mathcal{U}[U^*]$.

This corollary includes the known result that single unknown unitary is sufficient for the case $d = 2$. The encoder and decoder defined by Eqs. (4.27) coincide with $\mathcal{U}[\sigma_y]$. Thus in the 2-dimensional case we recover Eq. (2.24). Corollary 15 further reveals a significant difference between state transposition and unitary conjugation for higher dimensional systems. Unlike clones for state transposition, replicas of unitaries are helpful for unitary conjugation. State transposition and channel transposition behave differently according to the types of added non-linearity.

Corollary 15 states that $d-1$ replicas of the unknown unitary is sufficient for unitary conjugation. We do not know, however, if $d-1$ replicas are also necessary for this purpose. We are only sure that $2 = 3 - 1$ replicas are necessary for

3-dimensional case, since Thm. 11 denies probabilistic realisability without replication. The pair of encoder and decoder has plenty of room for improvement. The presented method does not make use of an additional ancillary system $\mathcal{H}_A$, and the replicated unitaries are used only in parallel. It is an interesting open problem to see if we can reduce the number of replicas required.

Theorem 13 tells us that on antisymmetric subspace, conjugated unitary $\mathcal{U}[U^{*\otimes n}]$ is implementable sometimes from smaller number of unknown unitaries $\mathcal{U}[U^{\otimes m}]$ with $m \leq n$. Anti-symemtric subspaces have a special feature with regard to conjugation. In the next subsection, we interpret this feature from the relation between particles and holes in fermion systems.

We close this subsection with a comment on computation of conjugation induced quantities. Although we have shown that finite replicas of unitary channels is sufficient for unitary conjugation, our encoding scheme requires a $\dim \mathcal{H}^{\otimes d-1} = d^{d-1}$ dimensional system to conjugate unitaries. This scales so rapidly according to the original system size d. The combination of our unitary conjugation method and the direct estimation of state overlap we reviewed in Sec. 2.3.4 does not seem to provide an efficient method to compute conjugation induced quantities. Our analysis on unitary conjugation, however, can be applied to another computation method presented in Sec. 4.3.

Remark 16. Corollary 15 has a simple group theoretic interpretation. It is known that for the defining representation R of $\mathrm{SU}(d)$, its conjugate representation R^* appears as an irreducible block of $R^{\otimes d-1}$. Although R^* and $R^{\otimes d-1}$ are not unitarily equivalent for $d \geq 2$, we can subtract R^* from $R^{\otimes d-1}$ by applying an appropriate encoding scheme with $\mathcal{E}$ and $\mathcal{D}$.

Remark 17. As already mentioned, the encoder and decoder for 2-dimensional unitary conjugation coincides with $\mathcal{U}[\sigma_y]$. For a 2-dimensional case, random unitary channels defined by

$$\sum_i p_i \, \mathcal{U}[U_i] \tag{4.31}$$

for a set of unitaries U_i and probability p_i, can be transposed by the same encoder and the decoder:

$$\begin{aligned} \mathcal{U}[\sigma_y] \circ \left(\sum_i p_i \, \mathcal{U}[U_i] \right) \circ \mathcal{U}[\sigma_y] &= \sum_i p_i \left(\mathcal{U}[\sigma_y] \circ \mathcal{U}[U_i] \circ \mathcal{U}[\sigma_y] \right) && (4.32) \\ &= \sum_i p_i \, \mathcal{U}[U_i^*] && (4.33) \\ &= \mathrm{T} \circ \left(\sum_i p_i \, \mathcal{U}[U_i] \right) \circ \mathrm{T}. && (4.34) \end{aligned}$$

This is not the case for our encoding scheme for $d \geq 3$-dimensions, since the unitaries may not act collectively. We rather need collective random unitary channels of the form

$$\sum_i p_i \, \mathcal{U}[U_i^{\otimes d-1}] \tag{4.35}$$

to implement the d-dimensional transposed random unitary channels

$$\mathrm{T} \circ \left(\sum_i p_i \, \mathcal{U}[U_i] \right) \circ \mathrm{T} = \mathcal{D} \circ \left(\sum_i p_i \, \mathcal{U}[U_i^{\otimes d-1}] \right) \circ \mathcal{E}. \tag{4.36}$$

4.2.3 Physical interpretation of unitary conjugation with replicas

In this subsection we identify antisymmetric subspaces and fermion systems, and interpret Thm. 13 in terms of fermions[3]. Anti-symmetric subspace $\mathcal{H}^{\wedge n}$ of $\mathcal{H}^{\otimes n}$ is equivalent to the n-particle subspace of a fermion system whose internal degree of freedom is $d = \dim \mathcal{H}$, under the identification

$$|\wedge_{i_1,\ldots,i_n}\rangle \sim |\Psi^{\text{particle}}_{i_1,\ldots,i_n}\rangle := a^\dagger_{|i_1\rangle} \ldots a^\dagger_{|i_n\rangle} |\text{vac}\rangle. \tag{4.37}$$

Here $a_{|j\rangle}$ represents the annihilation operator that erases a fermion in state $|j\rangle$, and $|\text{vac}\rangle$ represents the vacuum state $a_{|i\rangle}|\text{vac}\rangle = 0$ $(\forall i)$.

If $m + n = d$, the antisymmetric subspace $\mathcal{H}^{\wedge m}$, equivalent to an m-particle subspace, is also equivalent to an n-hole subspace. The vacuum state for holes is the completely occupied state for the particle defined by

$$|\text{occ}\rangle := a^\dagger_{|1\rangle} \ldots a^\dagger_{|d\rangle} |\text{vac}\rangle. \tag{4.38}$$

The operator creating (annihilating) a hole in state $|\psi\rangle$ is $a_{|\psi\rangle}$ $(a^\dagger_{|\psi\rangle})$. The roles of creation and annihilation operators are interchanged between particles and holes.

Under Eq. (4.37), the operator $A_{n\to m}$ is (up to phase) identified with an operator from the n-particle subspace to the $n(= d - m)$-hole subspace represented by

$$E^d_n := \sum_{1 \le i_1 < \ldots < i_n \le d} |\Psi^{\text{hole}}_{i_1,\ldots i_n}\rangle \langle \Psi^{\text{particle}}_{i_1,\ldots,i_n}|, \tag{4.39}$$

where

$$|\Psi^{\text{hole}}_{i_1,\ldots,i_n}\rangle := a_{|i_1\rangle} \ldots a_{|i_n\rangle} |\text{occ}\rangle.$$

See Appx. B.3 for the proof. Note that the operator E^d_n depends on the basis $\{|i\rangle\}_{i=1,\ldots,d}$. We call E^d_n a "particle-hole exchange operator".

Now we show how the encoder $\mathcal{E}$ and decoder $\mathcal{D}$ defined by Eq. (4.27) realise Thm. 13 in the picture of a fermion system. Figure 4.2 would help understanding the outline. Any n-particle fermion pure state is decomposable to the left hand side of Eq. (4.40). First, the action of encoder, represented by $\mathcal{U}[A_{n\to m}]$ on antisymmetric states, is equivalent to sending particle states to corresponding hole states:

$$\sum_{1 \le i_1 < \ldots < i_n \le d} \alpha_{i_1,\ldots,i_n} |\Psi^{\text{particle}}_{i_1,\ldots,i_n}\rangle \mapsto \sum_{1 \le i_1 < \ldots < i_n \le d} \alpha_{i_1,\ldots,i_n} |\Psi^{\text{hole}}_{i_1,\ldots,i_n}\rangle. \tag{4.40}$$

[3]Observations made in Sec. 4.2.3 are presented in Ref. [84]

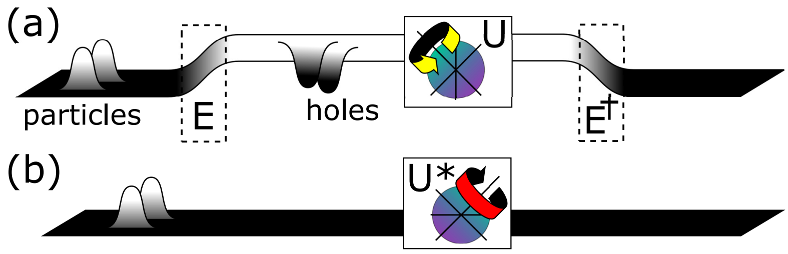

Figure 4.2: (a) The sequence of processes given in the left hand side of Eq. (4.25), presented in a fermion system. The encoder and the decoder interchanges particle and holes. All particles are transformed by U on $\mathcal{H}$ simultaneously. (b) The process equivalent to the one presented in (a).

The collective action $\mathcal{U}[U^{\otimes m}]$ of the unitary channel is equivalent to the mode transformation U on the n-hole (m-particle) space. The annihilation $a_{|i\rangle}$ and creation $a^\dagger_{|i\rangle}$ operators change according to the mode transformation respectively by

$$a^\dagger_{|i\rangle} \mapsto a^\dagger_{U|i\rangle} = \sum_{j=1}^{d} [U]_{ij} a^\dagger_{|j\rangle}, \tag{4.41}$$

$$a_{|i\rangle} \mapsto a_{U|i\rangle} = \sum_{j=1}^{d} [U]^*_{ij} a_{|j\rangle}. \tag{4.42}$$

Equation (4.42) implies that the hole state represented by the right-hand-side of Eq. (4.40) is transformed by the mode transformation according to

$$\sum_{1\le i_1<\ldots<i_n\le d} \alpha_{i_1,\ldots,i_n} |\Psi^{\text{hole}}_{i_1,\ldots,i_n}\rangle \tag{4.43}$$

$$\mapsto \sum_{1\le i_1<\ldots<i_n\le d} \sum_{j_1,\ldots,j_n=1}^{d} \alpha_{i_1,\ldots,i_n} [U]^*_{i_1 j_1} \cdots [U]^*_{i_n j_n} |\Psi^{\text{hole}}_{j_1,\ldots,j_n}\rangle. \tag{4.44}$$

The decoder sends this hole state back to the corresponding particle state:

$$\sum_{1\le i_1<\ldots<i_n\le d} \sum_{j_1,\ldots,j_n=1}^{d} \alpha_{i_1,\ldots,i_n} [U]^*_{i_1 j_1} \cdots [U]^*_{i_n j_n} |\Psi^{\text{hole}}_{j_1,\ldots,j_n}\rangle \tag{4.45}$$

$$\mapsto \sum_{1\le i_1<\ldots<i_n\le d} \sum_{j_1,\ldots,j_n=1}^{d} \alpha_{i_1,\ldots,i_n} [U]^*_{i_1 j_1} \cdots [U]^*_{i_n j_n} |\Psi^{\text{particle}}_{j_1,\ldots,j_n}\rangle. \tag{4.46}$$

The final state is equivalent to the original state changed by the mode transformation U^* *on particles*. This mode transformation is represented by the collective action $U^{*\otimes n}$ of n replicas of U^* on the antisymmetric subspace $\mathcal{H}^{\wedge n}$ of $\mathcal{H}^{\otimes n}$.

In summary, the encoder sends particle states to their corresponding hole states, and the decoder sends them back to particle states. If a mode transformation U is performed on the intermediate hole states, it is equivalent to performing mode transformation U^* on the particle state. Theorem 13 is obtained by reinterpreting this fact in the antisymmetric subspaces.

Remark 18. An operator connecting particle space and hole space is considered in nuclear shell theory and is called "particle-hole conjugation" [86, 87, 88]. The operator E_n^d differs from the particle-hole conjugation but is related to it. Let j be a total angular momentum of a shell and

$$a_{|m\rangle},\ (m = j,\ j-1, ...,\ \ -j) \tag{4.47}$$

be the annihilation operators of the particles spanning the shell. The particle-hole conjugation operator C is a unitary operator on the Fock space $\oplus_{n=0}^{d}\mathcal{H}^{\wedge n}$ defined by

$$C|\mathrm{vac}\rangle = a^\dagger_{|j\rangle}a^\dagger_{|j-1\rangle}...a^\dagger_{|-j\rangle}|\mathrm{vac}\rangle =: |\mathrm{occ}\rangle, \tag{4.48}$$

$$Ca^\dagger_{|m\rangle}a^\dagger_{|n\rangle}...|\mathrm{vac}\rangle = (-1)^{m+j}a_{|-m\rangle}(-1)^{n+j}a_{|-n\rangle}...|\mathrm{occ}\rangle, \tag{4.49}$$

for any different $m, n, ... \in \{j,\ j-1, ...,\ \ -j\}$ [87]. Equation (4.49) reveals that the action of C on the n-particle subspace is represented by

$$C|_{n-particle} = \sum_{j\geq m_1>...>m_n\geq -j} (-1)^{nj+\sum_{i=1}^n m_i}|\Psi^{\mathrm{hole}}_{-m_1,...,-m_n}\rangle\langle\Psi^{\mathrm{particle}}_{m_1,...,m_n}|. \tag{4.50}$$

The action of C on the n-particle subspace is represented by a particle-hole exchange operator followed (preceded) by a unitary operator on the n-hole (n-particle) subspace.

Remark 19. The name "particle-hole conjugation" might remind some readers with a different operator C' on the Fock space than C, whose action is represented by

$$C'a_{|\psi\rangle}C'^\dagger = a^\dagger_{|\psi\rangle},\ C'a^\dagger_{|\psi\rangle}C'^\dagger = a_{|\psi\rangle} \tag{4.51}$$

for any single-particle state $|\psi\rangle \in \mathcal{H}$. This operator is different from the particle-hole conjugation C considered in nuclear shell theory, and is decomposed into

$$C' = \left(\oplus_{n=0}^d E_n^d\right)\Theta', \tag{4.52}$$

where Θ' is a complex conjugation in the basis $\{|\Psi^{\mathrm{particle}}_{i_1,...i_n}\rangle\}_{n=0,...,d;1\leq i_1<...<i_n\leq d}$. Interestingly, C' does not depend on the single-particle basis $\{|i\rangle\}_{i=1,...,d}$ while Θ' and the particle-hole exchange operators do.

4.3 Observables for conjugation induced quantities

In this section, the techniques developed for unitary conjugation is applied to computation of conjugation induced quantities[4]. Unitary conjugation is previously known to be possible for 2-dimensional unitaries by sandwiching the unknown unitary channel by $\mathcal{U}[\sigma_y]$, and we have generalised $\mathcal{U}[\sigma_y]$ to other CP map pairs

[4]The content of Sec. 4.3 is presented in Ref. [84]

to deal with conjugation of higher dimensional unitaries. The combination of conjugation and σ_y operator also appears in the definition of the concurrence (see Sec. 2.3.3 for details). This fact motivates us to look for an implication of our results on unitary conjugation to the analysis on conjugation induced quantities like concurrence.

We propose a unified treatment of conjugation induced quantities listed in Sec. 2.3.3 (except the relative entropy of $\mathcal{PT}$-symmetry), and a method to construct observables measuring them. With these observables, conjugation induced quantities can be evaluated on pure states without knowledges on their state description. The method provides a direct link between construction of observable entanglement measures presented in Ref. [80, 71] (see Sec. 2.3.4), and our encoder and decoder for the unitary conjugation. Our construction of observables generalises the one presented in Ref. [81] (see Sec. 2.3.4 for a review).

Let us start from defining a class of conjugation induced quantity generated by linear maps. In this section, we use symbol $\bullet$ to denote the tensor product between cloned states, to distinguish it from the tensor product $\otimes$ for partitioning of multipartite systems.

Definition 20 (S-concurrence)**.** Let m and n be positive integers and $S : \mathcal{B}(\mathcal{H}^{\bullet n}) \to \mathcal{B}(\mathcal{H}^{\bullet m})$ be a linear map. The S-concurrence $\mathrm{C}_S(\psi)$ for a pure state $|\psi\rangle \in \mathcal{H}$ is defined by

$$\mathrm{C}_S(\psi) := \langle\psi|^{\bullet m} S(|\psi^*\rangle\langle\psi^*|^{\bullet n})|\psi\rangle^{\bullet m}. \tag{4.53}$$

Once we define the S-concurrence by Eq. (4.53), the observable for the S-concurrence is immediately constructed by the Choi isomorphism. For the Choi operator $\widetilde{S} \in \mathcal{B}(\mathcal{H}^{\bullet n} \bullet \mathcal{H}^{\bullet m})$ of S[5], its defining property (1.16) implies

$$\begin{aligned}
\mathrm{C}_S(\psi) &= \mathrm{Tr}\left[|\psi\rangle\langle\psi|^{\bullet m} S(|\psi^*\rangle\langle\psi^*|^{\bullet n})\right] && (4.54)\\
&= \mathrm{Tr}\left[|\psi\rangle\langle\psi|^{\bullet m} \widetilde{S}(|\psi^*\rangle\langle\psi^*|^{\bullet n})^{\mathrm{T}}\right] && (4.55)\\
&= \mathrm{Tr}\left[|\psi\rangle\langle\psi|^{\bullet m+n} \widetilde{S}\right], = \langle\psi|^{\bullet m+n}\widetilde{S}|\psi\rangle^{\bullet m+n} && (4.56)
\end{aligned}$$

for any pure state $|\psi\rangle$. Equation (4.56) states that $\mathrm{C}_S(\psi)$ is obtained as the expectation value of the Choi operator $\widetilde{S}$ for cloned state $|\psi\rangle^{\bullet m+n}$. If $\widetilde{S}$ is a Hermitian operator, the S-concurrence is obtained by measurement of $\widetilde{S}$. This construction of observables recovers the one presented by Eq. (2.62) proposed in Refs. [82, 83] by restricting $m = n$ to 1 and S to a completely positive map. Note that C_S is non-negative if S is positive. Non-negativity is required for C_S if it should quantify certain resources such as entanglement and asymmetries, since the minimum value of $\mathrm{C}_S(\psi)$ must be set to 0 for the states not useful as resources.

In the special case where $n = m$ and the linear map is presented by $S = \mathcal{U}[O]$ with some Hermitian operator O, our observable $\widetilde{S} = \widetilde{\mathcal{U}[O]}$ coincides with the one

[5] Here we use symbol $\bullet$ also for the bipartition of the Choi operator to keep symbol $\otimes$ to denote partition of multipartite systems later. Bipartition of Choi operators and multipartite systems are different.

presented by Eq. (2.60) proposed in Ref. [81]. By a straightforward calculation, we obtain

$$\begin{aligned}\widetilde{\mathcal{U}[O]} &= \mathbb{I}_{\mathcal{H}} \bullet O \left(\sum_{ij} |i\rangle \bullet |i\rangle\langle j| \bullet \langle j| \right) \mathbb{I}_{\mathcal{H}} \bullet O^{\dagger} \\ &= \mathrm{T} \bullet \mathrm{id}_{\mathcal{H}} \left(\mathbb{I}_{\mathcal{H}} \bullet O \mathrm{SWAP}_{\mathcal{H}\bullet\mathcal{H}} \mathbb{I}_{\mathcal{H}} \bullet O^{\dagger} \right) \\ &= \mathrm{T} \bullet \mathrm{id}_{\mathcal{H}} \left(O \bullet O^{\dagger} \mathrm{SWAP}_{\mathcal{H}\bullet\mathcal{H}} \right),\end{aligned}$$

which is equal to Eq. (2.60) when O is Hermitian. The second equality follows from Eq. (2.3).

We show a condition on S so that C_S is a local unitary invariant. For simplicity we consider a bipartite system $\mathcal{H}_A \otimes \mathcal{H}_B$, but the multipartite generalisation is straightforward. For an S-concurrence to be invariant under local unitary channel $\mathcal{U}[U_A \otimes U_B]$,

$$\begin{aligned}& \mathrm{C}_S(U_A \otimes U_B \psi) \\ =\ & \mathrm{Tr}\left[(\mathcal{U}[U_A \otimes U_B](|\psi\rangle\langle\psi|))^{\bullet m} S((\mathcal{U}[U_A \otimes U_B](|\psi\rangle\langle\psi|))^{*\bullet n})\right] \\ =\ & \mathrm{Tr}\left[|\psi\rangle\langle\psi|^{\bullet m} \mathcal{U}[(U_A \otimes U_B)^{\dagger\bullet m}] \circ S \circ \mathcal{U}[(U_A \otimes U_B)^{*\bullet n}](|\psi\rangle\langle\psi|^{*\bullet n})\right] \\ =\ & \mathrm{C}_{\mathcal{U}[(U_A\otimes U_B)^{\dagger\bullet m}]\circ S \circ \mathcal{U}[(U_A\otimes U_B)^{*\bullet n}]}(\psi)\end{aligned}$$

must be equal to $\mathrm{C}_S(\psi)$ for any state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$. This is satisfied if

$$S = \mathcal{U}[(U_A \otimes U_B)^{\dagger\bullet m}] \circ S \circ \mathcal{U}[(U_A \otimes U_B)^{*\bullet n}] \tag{4.57}$$

for all unitary operators U_A and U_B. In terms of the Choi operator $\widetilde{S}$, Eq. (4.57) is rewritten into

$$\widetilde{S} = U_A^{\dagger\bullet m+n} \otimes U_B^{\dagger\bullet m+n} \widetilde{S} U_A^{\bullet m+n} \otimes U_B^{\bullet m+n}, \tag{4.58}$$

in exactly the same way we have done for the case $n = m = 1$ in Rem 12. Thus we have found the symmetry of observables (2.63) considered first by Mintert [80], from the requirement that the conjugation induced quantity is invariant under local unitary channels. Although Mintert's method is not aimed for constructing observables from given conjugation induced quantities, our method provides observables once the linear maps S are given.

In the remainder of this section, we express known quantities reviewed in Sec. 2.3.3 as S-concurrences. The linear maps S are already known for the I-concurrence, and easily derived for filter based quantities, such as the Θ-concurrence and the asymmetry measure. We find new expression for the G-concurrence and related concurrence monotones whose conjugation based expression were not known.

4.3.1 Example: Θ-concurrence, asymmetry measures, filter based quantities

Perhaps the easiest examples are those quantities represented by

$$|\langle\psi|^{\bullet n} O \Theta |\psi\rangle^{\bullet n}| = \sqrt{\langle\psi|^{\bullet n} \mathcal{U}[O](|\psi^*\rangle\langle\psi^*|^{\bullet n})|\psi\rangle^{\bullet n}} = \sqrt{\mathrm{C}_{\mathcal{U}[O]}}, \tag{4.59}$$

with some operator O on $\mathcal{H}^{\bullet n}$. In these cases the linear map S is $\mathcal{U}[O]$ which is CP because they are already in the Kraus decomposition form. If O is Hermitian, the observables for these conjugation induced quantities coincides with the one proposed in Ref. [81], and this is the case for the Θ-concurrence, $\mathcal{PT}$-asymmetry measures, and filter based quantities.

The simplest one is the Θ-concurrence

$$\mathrm{C}_\Theta(|\psi\rangle) = |\langle\psi|\Theta|\psi\rangle| = \sqrt{\mathrm{C}_{\mathrm{id}_\mathcal{H}}(|\psi\rangle)}. \tag{4.60}$$

Thus the observable for the Θ-concurrence is $\widetilde{\mathrm{id}_\mathcal{H}} = \Phi_{\mathcal{H}\bullet\mathcal{H}}$, the density operator of the unnormalised maximally entangled vector given by $\sum_i |i\rangle \bullet |i\rangle$. We obtain

$$\mathrm{C}_\Theta(|\psi\rangle) = \sqrt{\mathrm{Tr}[|\psi\rangle\langle\psi|^{\bullet 2}\Phi_{\mathcal{H}\bullet\mathcal{H}}]} = |\langle\psi|^{\bullet 2}\sum_i |i\rangle^{\bullet 2}|. \tag{4.61}$$

Skew-information and the fidelity measure of $\mathcal{PT}$-symmetry are both calculated by $|\langle\psi|P\Theta|\psi\rangle| = \sqrt{\mathrm{C}_{\mathcal{U}[P]}}$. If $\widetilde{\mathcal{U}[P]}$ represents the Choi operator for $\mathcal{U}[P]$,

$$\sqrt{\mathrm{C}_{\mathcal{U}[P]}} = \sqrt{\mathrm{Tr}[|\psi\rangle\langle\psi|^{\bullet 2}\widetilde{\mathcal{U}[P]}]}. \tag{4.62}$$

Although the authors of Ref. [39] considered a method to compute these measures of $\mathcal{PT}$-asymmetry by using the combination of embedding quantum simulator and direst estimation of overlaps between states (see Sec. 2.3.4 for details), we find that they are more easily computed from expectation values of a certain observable.

The simplest example of the filter based quantity would be the qubit concurrence where $n = 1$ and $O = \sigma_y \otimes \sigma_y$. We postpone the analysis on qubit concurrence until the I-concurrence which coincides with qubit concurrence when $\dim \mathcal{H} = 2$.

4.3.2 Example: I-concurrence

The linear map S for the bipartite I-concurrence is

$$S = S'^{\otimes 2} = \left(\nu_d \sum_{1\le j<k\le d} \mathcal{U}[\frac{-i}{\sqrt{2}}(|j\rangle\langle k| - |k\rangle\langle j|)]\right)^{\otimes 2}, \tag{4.63}$$

which is already obtained in Ref. [75] (see Sec. 2.3.3 for a short review). Since S is a completely positive map with single input and single output, Eq. (2.62) presented in Refs. [82, 83] already provides the Choi operator as an observable. The Choi operator for $S'^{\otimes 2} : \mathcal{B}(\mathcal{H}\otimes\mathcal{H}) \to: \mathcal{B}(\mathcal{H}\otimes\mathcal{H})$ is a product of those for $S' : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ given by

$$\widetilde{S'} = \nu_d^2 \sum_{1\le j<k\le \dim\mathcal{H}} |\wedge_{j,k}\rangle\langle\wedge_{j,k}| = \nu_d^2 \Pi_{\mathcal{H}^{\wedge 2}}, \tag{4.64}$$

where $|\wedge_{j,k}\rangle$ is defined by Eq. (4.24), and $\Pi_{\mathcal{H}^{\wedge 2}}$ is the projector onto the antisymmetric subspace $\mathcal{H}^{\wedge 2}$ of $\mathcal{H}^{\bullet 2}$. Thus we obtain

$$\mathrm{C}_I(|\psi\rangle\langle\psi|) = \mathrm{C}_{S'\otimes S'}(|\psi\rangle\langle\psi|) = \nu_d^4 \mathrm{Tr}[|\psi\rangle\langle\psi|^{\bullet 2}\Pi_{\mathcal{H}^{\wedge 2}} \otimes \Pi_{\mathcal{H}^{\wedge 2}}]. \tag{4.65}$$

In the next example we find the G-concurrence and related concurrence monotones by generalising the superoperator projector S'.

4.3.3 Example: G-concurrence and related family of quantities

Now, we consider an example of linear map S which has not been considered before. Remember that the operator $\mathcal{U}[A_{n\to m}]$ satisfies the symmetry (4.29). This symmetry is generalised to the case $n+m \not\leq d$ with modifications on $\mathcal{U}[A_{n\to m}]$. These modified CP maps define a family of concurrence monotones presented in Ref. [69] (see Sec. 2.3.2).

First define operators $A_{i_1,\ldots,i_{n+m}}$ by

$$A_{i_1,\ldots,i_{n+m}} : \mathcal{H}^{\bullet n} \to \mathcal{H}^{\bullet m} \tag{4.66}$$

$$A_{i_1,\ldots,i_{n+m}} = \frac{1}{\sqrt{(n+m)!}} \sum_{\tau\in \mathrm{S}_{n+m}} \mathrm{sgn}(\tau)|\tau_{i_1},\ldots,\tau_{i_n}\rangle\langle\tau_{i_{n+1}},\ldots,\tau_{i_{n+m}}| \tag{4.67}$$

for $1 \leq i_1 < \ldots < i_{n+m} \leq d$. Operator $A_{i_1,\ldots,i_{n+m}}$ coincides with $\frac{n!m!}{(m+n)!}A_{n\to m}$ when $n+m=d$, and is defined even in the case $n+m \not\leq d$. Let $S' : \mathcal{B}(\mathcal{H}^{\bullet n}) \to \mathcal{B}(\mathcal{H}^{\bullet m})$ be the CP map whose Kraus operators are $A_{i_1,\ldots,i_{n+m}}$, namely,

$$S' = \sum_{1\leq i_1<\ldots<i_{n+m}\leq d} \mathcal{U}[A_{i_1,\ldots,i_{n+m}}]. \tag{4.68}$$

The Choi operator $\widetilde{S'}$ for S' is the projector

$$\widetilde{S'} = \Pi_{\mathcal{H}^{\wedge n+m}} = \sum_{1\leq i_1<\ldots<i_{m+n}\leq d} |\wedge_{i_1,\ldots,i_{m+n}}\rangle\langle\wedge_{i_1,\ldots,i_{m+n}}|. \tag{4.69}$$

onto the antisymmetric subspace $\mathcal{H}^{\wedge n+m}$ of $\mathcal{H}^{\otimes n+m}$ (see Appx. B.1). Thus the observable for a bipartite quantity $\mathrm{C}_{S'\otimes S'}$ is $\Pi_{\mathcal{H}^{\wedge n+m}}$, which is known to measure C^G_{n+m} by Eq. (2.65) [71]. The local unitary invariance of C^G_{n+m} is expressed by the invariance $\widetilde{S'} = U^{\dagger\bullet n+m}\widetilde{S'}U^{\bullet n+m}$ of the observable [80, 71] which we show is equivalent to the symmetry $\mathcal{U}[U^{*\bullet m}] \circ S' = S' \circ \mathcal{U}[U^{\bullet n}]$ of the linear map S' (see Rem. 12). The conjugation induced quantities inspired by the unitary conjugation algorithm, and the observable local unitary invariants are equivalent in this way.

For a mixed state $\rho \in \mathcal{S}(\mathcal{H}\otimes\mathcal{H})$, $\mathrm{C}_{S'\otimes S'}(\rho)$ does not necessarily measure correlation between the bipartition. For bipartite product mixed state $\rho_1\otimes\rho_2$, $\mathrm{C}_{S'\otimes S'}(\rho_1\otimes\rho_2)$ reduces to $\mathrm{C}_{S'}(\rho_1)\times \mathrm{C}_{S'}(\rho_2)$, where each component is

$$\mathrm{C}_{S'}(\rho_j) = \sum_{1\leq i_1<\ldots<i_{n+m}\leq d} p_{i_1}\ldots p_{i_{n+m}}, \tag{4.70}$$

with p_is as the probability eigenvalues of ρ_j (see Appx. B.2 for the proof). Since this value evaluates how mixed the state is, $\mathrm{C}_{S'\otimes S'}$ measures not only bipartite correlation but also mixedness, if applied on mixed states.

Chapter 5

Composite systems in topos quantum theory

We have investigated the behaviour of the gap between positive and CP maps starting from quantum theory in previous two chapters. In the subsequent two chapters, in contrast, we start from classical probability theory and investigate the gap between positive and CP maps in topos quantum theory. Topos quantum theory provides a representation of quantum states as direct generalisations of probability distributions, namely valuation (see Sec. 5.1.1 for more details).

In this chapter, we focus on composite systems in topos quantum theory. So far topos quantum theory has been mainly considered only for a single system and there remains much unexplored in composite systems, while these are intensively studied in usual quantum theory formalised by Hilbert spaces. Analysis on composite systems is expected to reveal significant for the gap between positive and CP maps in topos quantum theory, since the defining difference between positive and CP maps appear in composite systems as we have reviewed in Sec. 1.1.

Specifically, we generalise the definition of composite systems in classical probability to topos quantum theory, and analyse the correspondence between quantum states and valuations on composite systems. It turns out that the valuations corresponds to positive over pure tensor states, rather than quantum states. This has an implication on positivity in our definition of composite systems in topos quantum theory.

We first give an introduction to topos quantum theory and related category theory in Sec. 5.1. Then we define composite systems in topos quantum theory in Sec. 5.2. Finally in Sec. 5.3, we show the bijective correspondence between valuations on our composite systems and positive over pure tensor states, and analyse their difference from usual quantum states.

5.1 Introduction to topos quantum theory

In this section we give a short introduction of topos quantum theory. Familiarity on basic category theory would be helpful for proper understanding.

There are several branches in topos quantum theory. A basic idea common to all of them is to find quantum theory as a direct generalisation of classical probability theory by using topos. From a topos theory point of view, classical probability theory is a topos quantum theory formalised in the particluar topos **Sets**.

We briefly recall classical probability theory before moving on to topos. A random variable is represented by a finite set, say, X. A probability distribution p on X is a function $p : X \to [0,1]$ such that $\sum_{x \in X} p(x) = 1$. Equivalently, a probability distribution is an assignment of probability weights on measurable subsets of X. If the set of subsets of the finite set X is denoted by $\mathrm{Sub}(X)$, the assignment is a function $p : \mathrm{Sub}(X) \to [0,1]$ satisfying conditions

$$p(X) = 1, \; p(\emptyset) = 0, \tag{5.1}$$

$$p(V) \leq p(W) \text{ if } V \subset W \text{ in } \mathrm{Sub}(X), \tag{5.2}$$

$$p(V) + p(W) = p(V \cap W) + p(V \cup W), \tag{5.3}$$

where W and V are subsets of X.[1]

Topos quantum theory uses probability *valuations* to represent quantum states (we shall omit adjective "probability" since all valuations appearing in this thesis is normalised). Valuations are similar to probability measures, but differs especially in that they are defined on *locales*. A locale X is a certain lattice whose elements are called "opens". If a locale further has a certain structures of opens called "points," it is called a topological space. The set of subset of X, $\mathrm{Sub}(X)$ forms a topological space whose points corresponds to the elements of X. Locales in general do not necessarily have points. A valuation on a locale is an assignment of probability weights on the opens of the locale such that the conditions analogous to Eqs. (5.1), (5.2) and (5.3) are satisfied (see Sec. 5.1.1 for details).

Topos quantum theory differs from classical probability theory not only in the use of locales and valuations but also in the category on which they are defined. For defining concepts and proving theorems in classical probability theory, we usually use set-theoretic logic. Toposes are categories with associated languages which enables interpretation of formal logical expressions inside the toposes (see Appx. C.4.2 for detail). From topos theoretic point of view, set-theoretic logic is the language associated to topos **Sets**. We shall call mathematical concepts to be *internal* to a topos, if they are interpreted by the language of the topos.

Major branches of topos quantum theories [89, 90] start from finding proper toposes for a given Hilbert space $\mathcal{H}$ (or more generally, a non-commutative C*-algebra). Then internal locales are constructed so that valuations on them have one-to-one correspondence to quantum states on $\mathcal{H}$. We obtain the representation of quantum states by valuations in this way.

Table 5.1 summarises how topos quantum theory generalise probability theory to express quantum states. Since valuations are direct generalisations of probability distributions, we can ask how far the properties of probability distributions are inherited to valuations for topos quantum theory. In this thesis, we consider generalisation of composite systems in this chapter and of maps in Chap. 6, where Markov chains are studied instead of maps.

[1] If we consider probability distributions as probability measures on discrete sets, more natural choice of conditions would be Eq. (5.1) and the σ-additivity. The σ-additivity is equivalent to conditions (5.2) and (5.3).

	probability theory	topos quantum theory
system	random variable (set)	locale
weight function	probability distribution	valuation
composites	product	Chap. 5
maps	transition matrix	Chap. 6

Table 5.1: Analogous concepts in classical probability theory and topos quantum theory. Systems here refers to general objects on which weight functions are defined.

In this chapter, we consider composite systems in topos quantum theory. In probability theory, the composite of random variables X and Y is defined by its product $X \times Y$. A natural generalisation of this composition to topos quantum theory would be given by the product of locales. If the valuations on locales X and Y respectively correspond to quantum states on the associated Hilbert spaces $\mathcal{H}_X$ and $\mathcal{H}_Y$, a proper composition $X \times Y$ is expected to lead a bijective correspondence between valuations on $X \times Y$ and quantum states on $\mathcal{H}_X \otimes \mathcal{H}_Y$. Although there seem to be many ways to define a product locale, we here choose one and test if it describes the composite quantum system. It turns out that the valuations on our product locale has a bijective correspondence between positive over pure tensor states rather than quantum states.

Of course it is possible to construct the topos for $\mathcal{H}_X \otimes \mathcal{H}_Y$ regarded as a single system, and construct the locale $X_{\mathcal{H}_X \otimes \mathcal{H}_Y}$ whose valuations have bijective correspondence between quantum states on $\mathcal{H}_X \otimes \mathcal{H}_Y$. This method is not of our interest since it neither makes a composition in topos quantum theory or is motivated from the composition in probability theory.

Among several branches of topos quantum theory, we focus on one of the mainstreams called "Bohrification approach". The Bohrification approach makes full use of the languages associated to topos. Although the axiom of choice and the law of excluded middle are no longer valid in a general topos, any mathematical theorems proven *constructively* are interpreted to be valid in any topos. Constructively proven theorems contribute to showing the existence of the set of valuations corresponding to quantum states. Since proposers of the other mainstream "contravariant approach" do not make use of the internal language of toposes, constructively proven theorems are not necessarily interpretable by their approach. Our result presented in this chapter and the next are not applicable for the contravariant approach since we use several known theorems from constructive mathematics. We give detailed introductions to these constructively proven theorems in Sec. 5.1.1, and to the Bohrification approach in Sec. 5.1.2.

5.1.1 Constructive Gelfand duality and Riesz theorem

In this subsection, we introduce two known theorems from constructive mathematics which play significant roles in this chapter. The Gelfand duality is a celebrated result in theory of algebras. Classically it gives a duality between commutative C*-algebras and compact Hausdorff spaces both internal to **Sets**, and constructive proofs extended the duality between general commutative C*-algebras and compact, completely regular locales. The Riesz theorem (also called Riesz-Markov theorem) expresses another duality relation between integrals over commutative C*-algebras and valuations on locales. Schematically, we shall explain following relation:

$$\begin{array}{ccc} \text{commutative C*-algebra } A & \dashrightarrow & \text{integrals over } A \\ {\scriptstyle \text{constructive Gelfand duality}} \updownarrow & & \updownarrow {\scriptstyle \text{constructive Riesz's theorem}} \\ \text{compact, completely regular locale } X & \dashrightarrow & \text{valuations on } X. \end{array} \tag{5.4}$$

The constructive Gelfand duality is represented by a contravariant equivalence between categories of commutative C*-algebras **cCstar** and compact, completely regular locales **KCRegLoc**. The proof of Gelfand duality to be constructive implies that this contravariant equivalence holds in any toposes. More precisely, we have following theorem:

Theorem 21. Let $\mathcal{T}$ be any topos and **cCstar** and **KCRegLoc** be categories of commutative C*-algebras and compact, completely regular locales defined internally to $\mathcal{T}$. There is a pair of contravariant functors Σ : **cCstar** $\rightarrow$ **KCRegLoc** and $\mathrm{Cont}(-,\mathbb{C})$: **KCRegLoc** $\rightarrow$ **cCstar** such that $\Sigma \circ \mathrm{Cont}(-,\mathbb{C})$ and $\mathrm{Cont}(-,\mathbb{C}) \circ \Sigma$ are the identity functors on **KCRegLoc** and **cCstar**, respectively.

This theorem is implied by the results presented in Ref. [48], and summarised in this form in Ref. [90]. In the following argument we do not specify the topos in question.

The compact completely regular locale $\Sigma_A := \Sigma(A)$ for an internal commutative C*-algebra A is called the *Gelfand spectrum* for A. Although there is a method to construct Σ_A from A, we can refer to the valuations on Σ_A without specifying the precise form of Σ_A. This is possible by combining the Gelfand duality and the Riesz theorem presenting a duality between following valuations and integrals.

A *valuation* on locale X is a morphism $v : \mathcal{O}(X) \rightarrow [0,1]$ such that

$$v(\bot) = 0, \tag{5.5}$$

$$v(\top) = 1 \qquad \text{(normalisation)} \tag{5.6}$$

$$v(U) + v(V) = v(U \vee V) + v(U \wedge V) \qquad \text{(the modular law)} \tag{5.7}$$

$$v(U) \leq v(V) \text{ if } U \leq V \text{ in } X \qquad \text{(monotonicity),} \tag{5.8}$$

for any opens U, V of X, where $\bot$ and $\top$ represents the bottom and top elements of X, respectively[2]. These conditions must be interpreted by internal languages of toposes.

An *integral* over a self-adjoint part C_{sa} of a C*-algebra C (we call it an integral over C for short) is formally defined as a morphism $I : C_{sa} \rightarrow \mathbb{R}$ such that

$$\begin{aligned} I(\mathbb{I}) &= 1 && \text{(normalisation),} \\ I(a+b) &= I(a) + I(b) && \text{(linearlity),} \\ I(a) &\geq 0 \text{ if } a \geq 0 && \text{(positivity)} \end{aligned} \tag{5.9}$$

[2]Precisely speaking, the morphism v is required to satisfy the following continuity: $\sup v(V_i) = v(\sup V_i)$ for directed family $\{V_i\}$. A family of opens $\{V_i\}$ is called directed if for any pair $V, W \in \{V_i\}$, there exists $X \in \{V_i\}$ such that $V \leq X$ and $W \leq V$.

hold for all $a, b \in C_{sa}$ and $\mathbb{I}$, the identity in C_{sa} [49] [3]. The conditions presented above should be interpreted by internal languages of toposes.

The constructive Riesz theorem states that there is a bijective correspondence between integrals over commutative C*-algebra A and valuations on the Gelfand spectrum Σ_A. Given an integral I, we can construct an associated valuation μ_I, and vice versa.

The constructive Riesz theorem states the equivalence not only of the integrals and valuations themselves, but also of the corresponding locales. Let 1 be the terminal object of internal locales. For each internal commutative C*-algebra A, there is an associated locale $\mathscr{I}A$ such that the set $\mathrm{Hom}_{\mathbf{Loc}}(1, \mathscr{I}A)$ has a bijective correspondence to integrals over A (see Appx. C.1 for the definition of "Hom"). For each internal locale X, there is an associated locale $\mathscr{V}X$ such that the set $\mathrm{Hom}_{\mathbf{Loc}}(1, \mathscr{V}X)$ has a bijective correspondence to valuations on X. The constructive Riesz theorem presented in Ref. [49] states the existence of the isomorphism

$$\mathscr{I}A \cong \mathscr{V}\Sigma_A, \tag{5.10}$$

in the category of locales, if commutative C*-algebra A and locale Σ_A are Gelfand dual. This implies an equivalence between $\mathrm{Hom}_{\mathbf{Loc}}(1, \mathscr{I}A)$ (integrals over A) and $\mathrm{Hom}_{\mathbf{Loc}}(1, \mathscr{V}\Sigma_A)$ (valuations on Σ_A). We do not write down the precise definitions of these locales here because it requires familiarity on logics (for interested readers, we recommend Ref. [91]), and because we only use several of their known properties which could be stated without their definitions.

Now in summary, the relation presented by the diagram (5.4) can be more precisely depicted by the following diagram:

$$\begin{array}{ccccc}
A \text{ in } \mathbf{cCstar} & \overset{\mathscr{I}}{\dashrightarrow} & \mathscr{I}A \text{ in } \mathbf{Loc} & \qquad & \mathrm{Hom}_{\mathbf{Loc}}(1, \mathscr{I}A) \cong \text{Integrals over } A \\
{\scriptstyle \mathrm{Cont}(-,\mathbb{C})}\uparrow\downarrow{\scriptstyle \Sigma} & & \Vert\wr & & \Vert\wr \\
\Sigma_A \text{ in } \mathbf{KCRegLoc} & \overset{\mathscr{V}}{\dashrightarrow} & \mathscr{V}\Sigma_A \text{ in } \mathbf{Loc}. & & \mathrm{Hom}_{\mathbf{Loc}}(1, \mathscr{V}\Sigma_A) \cong \text{Valuations on } \Sigma_A
\end{array} \tag{5.11}$$

The isomorphism (5.10) provides a way to analyse states in two ways. In this chapter, we show the one-to-one correspondence between positive over pure tensor states and integrals over algebras on composite systems. The isomorphism (5.10) then implies the one-to-one correspondence between positive over pure tensor states and valuations.

Example 22. As a simple example in **Sets**, let us consider $\mathrm{Cont}(\dot{2}, \mathbb{C})$, the continuous functions from a two element set $\dot{2} = \{x, y\}$ to $\mathbb{C}$. $\mathrm{Cont}(\dot{2}, \mathbb{C})$ forms a commutative C*-algebra in **Sets** with the element-wise summation and multiplication $f + g(z) := f(z) + g(z)$, $f \times g(z) := f(z)g(z)$ ($f, g \in \mathrm{Cont}(\dot{2}, \mathbb{C})$). In this example, $\dot{2}$ is the locale with the discrete topology, which is associated to $\mathrm{Cont}(\dot{2}, \mathbb{C})$ by the Gelfand duality.

The top three conditions for valuation v imply

$$v(\{x\}) + v(\{y\}) = v(\{x,\ y\}) + v(\emptyset) = 1. \tag{5.12}$$

[3] Most generally integrals are defined on f-algebras [49]. Here we only consider those f-algebras equivalent to self-adjoint parts of C*-algebras.

Thus v is completely determined by its value $v(\{x\}) \in [0,1]$ on $\{x\}$. In this classical example, valuations are equivalent to probability distributions. One can define the integral I_v associated to a valuation v by

$$I_v(f) := \sum_{z \in \dot{2}} f(z)v(z), \ (f : \dot{2} \to \mathbb{R}). \tag{5.13}$$

On the other hand, if an integral $I : \mathrm{Cont}(\dot{2}, \mathbb{R}) \to \mathbb{R}$ is given, the associated valuation v_I can be constructed by

$$v_I(x) = I(\chi_x), \ v_I(y) = I(\chi_y), \tag{5.14}$$

where χ_z are characteristic functions taking value 1 at z. These associations $I \mapsto v_I$ and $v \mapsto I_v$ are those indicated by the Riesz theorem.

5.1.2 Bohrification approach

In this subsection, we give a more detailed introduction to the Bohrification approach first presented in Ref. [90]. There are several branches inside the Bohrification approach [92, 93]. Among these sub-branches, we use the original approach for two reasons. First, the correspondence between quantum states and integrals or valuations has been most explicitly investigated in the original approach. Second, the internal language has a relatively simple form in the covariant functor topos $[P, \mathbf{Sets}]$ over poset P used in the original approach (see Appx. C.4.3 for details). For these two reasons, the original approach is suitable for starting the investigation of the composite systems.

Let A be a non-cmmutative algebra $\mathcal{B}(\mathcal{H})$ of bounded operators of a finite dimensional quantum system $\mathcal{H}$. Let $\mathcal{C}(A)$ be a poset of unital *commutative* subalgebras of A, ordered by the subalgebra inclusion, i.e. $C \leq D$ if and only if $C \subset D$. Each commutative C*-subalgebra C of a non-commutative C*-algebra A, namely, each element of poset $\mathcal{C}(A)$ is refered to as a "context".

The covariant approach uses the covariant functor topos $[\mathcal{C}(A), \mathbf{Sets}]$ for describing the quantum system A. The objects of $[\mathcal{C}(A), \mathbf{Sets}]$ are functors from poset $\mathcal{C}(A)$ to **Sets**, and morphisms are natural transformations between these functors.

The *Bohrification* of algebra A is the unital commutative C$^*-$algebra object $\underline{A}$ internal to $[\mathcal{C}(A), \mathbf{Sets}]$ defined by

$$\underline{A}(C) = C,$$

for each unital comutative C*-algebra $C \in \mathcal{C}(A)$. A unital commutative C*-algebra object in topos $\mathcal{T}$ is the object which satisfy axioms of unital commutative C*-algebras interpreted by the internal language of topos $\mathcal{T}$ (see Appx. C.4.2 for details).

It is shown in Ref. [90] that there is a bijective correspondence between the set of integrals over $\underline{A}$ internal to $[\mathcal{C}(A), \mathbf{Sets}]$, and the set of quasi-states on A, if the dimension of A is greater than 2. If $A = \mathcal{B}(\mathcal{H})$ for a finite dimensional Hilbert space $\mathcal{H}$ ($\dim\mathcal{H} \geq 3$), quasi-states on A are equivalent to density operators[4]. If the conditions for integrals are interpreted in $[\mathcal{C}(A), \mathbf{Sets}]$, an integral over $\underline{A}$ is a natural transformation $I : \underline{A}_{sa} \to \underline{\mathbb{R}}$, where $\underline{\mathbb{R}}$ is the real number object in $[\mathcal{C}(A), \mathbf{Sets}]$, such that each component $I_C : C_{sa} \to \mathbb{R}$ ($C \in \mathcal{C}(A)$) is an integral in **Sets** [90]. Given a density operator ρ, we can define the corresponding integral I_ρ by $I_{\rho C}(a) := \mathrm{Tr}[\rho a]$ ($\forall C \in \mathcal{C}(A)$, $\forall a \in C_{sa}$). Conversely, given an integral $I : \underline{A}_{sa} \to \underline{\mathbb{R}}$, we can define the corresponding density matrix ρ_I by $\mathrm{Tr}[\rho a] := I_C(a)$ ($\forall a \in A_{sa}$), where $C \in \mathcal{C}(A)$ is any context such that $a \in C_{sa}$. Once we have the equivalence between density operators and integrals, the equivalence between density operators and valuations immediately follows from the isomorphism (5.10).

5.2 Composite systems

In classical probability theory, if we have two spaces of random variables X and Y, their composition is the direct product $X \times Y$. The Gelfand duality suggests that taking the product of spaces X and Y is equivalent to taking the coproduct of corresponding algebras $\mathrm{Cont}(X, \mathbb{C})$ and $\mathrm{Cont}(Y, \mathbb{C})$, since we have

$$\mathrm{Cont}(X \times Y, \mathbb{C}) = \mathrm{Cont}(X, \mathbb{C}) \otimes \mathrm{Cont}(Y, \mathbb{C}), \tag{5.15}$$

where the tensor on the right hand side represents the coproduct. Thus the composition of classical systems is described by a product of spaces or, equivalently, a coproduct of algebras.

In this section, we consider composite systems in the Bohrification approach. We try to define composition by products of spectra and coproducts of algebras motivated from the definition of composition in classical probability theory. The generalisation is, however, not straightforward and we do not obtain the unique definition.

5.2.1 Coproducts of algebras

If A_i ($i = 1, ..., n$) are noncommutative C*-algebras describing independent systems $\mathcal{H}_i$, we have associated toposes $[\mathcal{C}(A_i), \mathbf{Sets}]$ and Bohrifications $\underline{A_i}$ each internal to $[\mathcal{C}(A_i), \mathbf{Sets}]$. An obstacle in forming a coproduct of algebras $\underline{A_i}$ is that the toposes in which they are defined are different. In Ref. [47], two unital commutative C*-algebras $\underline{A_1}$ in $[\mathcal{C}(A_1), \mathbf{Sets}]$ and $\underline{A_2}$ in $[\mathcal{C}(A_2), \mathbf{Sets}]$ are mapped to topos $[\mathcal{C}(A_1) \times \mathcal{C}(A_2), \mathbf{Sets}]$ by certain morphisms and composed there. We follow this technique and present it in the way applicable for coproducts of more than three algebras.

Let $\mathcal{C}(A_1) \times ... \times \mathcal{C}(A_n)$ be a product of posets $\{\mathcal{C}(A_i)\}_{i=1,...,n}$. There is a functor $f_i^* : [\mathcal{C}(A_i), \mathbf{Sets}] \to [\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Set}]$ defined by

$$f_i^* F(C_1, ..., C_n) = F(C_i), \qquad ((C_1, ..., C_n) \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n)) \tag{5.16}$$

[4]A quasi-state on A is a map $\rho : A \to \mathbb{C}$ that is positive and linear on all commutative subalgebras and satisfies $\rho(a + ib) = \rho(a) + i\rho(b)$ for all self-adjoint $a, b \in A$ (possibly non-commuting). If A is a von Neumann algebra and does not contain a type-II von Neumann factor, quasi-states are just usual quantum states. In particular, A does not contain type-II von Neumann factor if $A = \mathcal{B}(\mathcal{H})$ for certain finite dimensional Hilbert space $\mathcal{H}$.

for each objects F in $[\mathcal{C}(A_i), \mathbf{Sets}]$, which is itself a functor from $\mathcal{C}(A_i)$ to $\mathbf{Sets}$[5]. If f_i^* is applied on internal C*-algebra $\underline{A_i}$, object $f_i^* \underline{A_i}$ is a unital commutative C*-algebra internal to $[\prod_{i=1}^n \mathcal{C}(A_i),\ \mathbf{Set}]$ given by

$$f_i^* \underline{A_i}(C_1, ..., C_n) = C_i. \tag{5.17}$$

We define the C*-algebra of the composite system in topos quantum theory by the coproduct of $f_i^* \underline{A_i}$.

Theorem 23. [95] Denote the coproduct of $f_i^* \underline{A_i}$ $(i = 1, ..., n)$ in $\mathbf{cCstar}_{[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Set}]}$ by $f_1^* \underline{A_1} \otimes ... \otimes f_n^* \underline{A_n}$. As an object of $[\prod_{i=1}^n \mathcal{C}(A_i),\ \mathbf{Set}]$, $f_1^* \underline{A_1} \otimes ... \otimes f_n^* \underline{A_n}$ is explicitly given by

$$f_1^* \underline{A_1} \otimes ... \otimes f_n^* \underline{A_n}(C_1, ..., C_n) = C_1 \otimes ... \otimes C_n, \tag{5.18}$$

for $(C_1, ..., C_n) \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n)$, where the tensor product on the right hand side is for commutative C*-algebras in $\mathbf{Sets}$.

Proof. See Appx. D.1. □

It is already shown that Eq. (5.18) defines the coproduct when $n = 2$ [47]. We straightforwardly reinforced their result to coproducts of finitely many C*-algebras.

In summary, from the pairs of toposes and the Bohrification algebras in them $([\mathcal{C}(A_i), \mathbf{Sets}], \underline{A_i})$ $(i = 1, ..., n)$, we first make topos $[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Sets}]$. Its internal commutative C*-algebra $f_1^* \underline{A_1} \otimes ... \otimes f_n^* \underline{A_n}$ is obtained by taking the coproduct of $f_i^* \underline{A_i}$ $(i = 1, ..., n)$ in the cateogry of commutative C*-algebras internal to $[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Sets}]$. The explicit description of $f_1^* \underline{A_1} \otimes ... \otimes f_n^* \underline{A_n}$ is presented in Eq. (5.18).

5.2.2 Gelfand duality and products of spectra

Let $\underline{\Sigma}_{f_i^* \underline{A_i}}$ be the spectrum for $f_i^* \underline{A_i}$ obtained by the Gelfand duality in topos $[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Sets}]$. These spectra are related to the spectrum for the coproduct $f_1^* \underline{A_1} \otimes ... \otimes f_n^* \underline{A_n}$ by

$$\underline{\Sigma}_{f_1^* \underline{A_1} \otimes ... \otimes f_n^* \underline{A_n}} \cong \underline{\Sigma}_{f_1^* \underline{A_1}} \times ... \times \underline{\Sigma}_{f_n^* \underline{A_n}}, \tag{5.19}$$

since the contravariant equivalence $\Sigma_{(-)}$ changes coproducts in $\mathbf{cCstar}_{[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Sets}]}$ into producs in $\mathbf{KCRegLoc}_{[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Sets}]}$.

There is a different way to take the product of Gelfand spactra, which gives an object not necessarily equal to $\underline{\Sigma}_{f_1^* \underline{A_1}} \times ... \times \underline{\Sigma}_{f_n^* \underline{A_n}}$. If the geometric morphisms f_i^* are applied to spectra $\underline{\Sigma}_{A_i}$, the resulting objects $f_i^* \underline{\Sigma}_{A_i}$ are compact regular locales internal to $[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Sets}]$[6]. The compact regular locale $f_i^* \underline{\Sigma}_{A_i}$ is not necessarily equal to $\underline{\Sigma}_{f_i^* \underline{A_i}}$. In other words, the following diagram does not necessarily

[5] A class of functors between toposes called *geometric morphisms* play central roles in topos theory. Functor f_i^* defined here is a geometric morphism from $[\mathcal{C}(A_i), \mathbf{Sets}]$ to $[\prod_{i=1}^n \mathcal{C}(A_i),\ \mathbf{Set}]$ [47]. See e.g. Ref. [94] for details of geometric morphisms.

[6] This is because the theory of Gelfand spectrum is geometric [48], and the Gelfand spectra is preserved by the geometric morphisms.

commute:

$$\begin{array}{ccc} \mathbf{cCstar}_{[\mathcal{C}(A_i),\mathbf{Sets}]} & \xrightarrow{\Sigma} & \mathbf{KCRegLoc}_{[\mathcal{C}(A_i),\mathbf{Sets}]} \\ \downarrow f_i^* & & \downarrow f_i^* \\ \mathbf{cCstar}_{[\prod_{i=1}^n \mathcal{C}(A_i),\mathbf{Sets}]} & \xrightarrow{\Sigma} & \mathbf{KCRegLoc}_{[\prod_{i=1}^n \mathcal{C}(A_i),\mathbf{Sets}]}. \end{array} \tag{5.20}$$

Therefore their product $f_1^*\underline{\Sigma}_{\underline{A_1}} \times ... \times f_n^*\underline{\Sigma}_{\underline{A_n}}$ taken in $\mathbf{KCRegLoc}_{[\prod_{i=1}^n \mathcal{C}(A_i),\mathbf{Sets}]}$ is not necessarily equal to $\underline{\Sigma}_{f_1^*\underline{A_1}} \times ... \times \underline{\Sigma}_{f_n^*\underline{A_n}}$.

Although $f_1^*\underline{\Sigma}_{\underline{A_1}} \times ... \times f_n^*\underline{\Sigma}_{\underline{A_n}}$ may differ from $\underline{\Sigma}_{f_1^*\underline{A_1}} \times ... \times \underline{\Sigma}_{f_n^*\underline{A_n}}$, it is another definition of composite systems in the Bohrification approach generalising the composition of classical systems. The fact that there is no unique way to extend the definition of composition to the Bohrification approach (and in fact, to any topos quantum theory) stems from the different toposes for marginal systems. In classical measure theory, any marginal systems are objects in the unified topos **Sets**. In the topos quantum theory, marginal systems are equipped with their own toposes. When taking the coproduct of algebras or product of spectra, we need to send them to a unified topos by properly chosen maps such as geometric morphisms. Then the ambiguity arises from the non-commutativity of the diagram (5.20).

The remainder of this thesis only concerns the composite systems defined by the coproduct $f_1^*\underline{A_1} \otimes ... \otimes f_n^*\underline{A_n}$ and product $\underline{\Sigma}_{f_1^*\underline{A_1}} \times ... \times \underline{\Sigma}_{f_n^*\underline{A_n}}$. To simplify notations, we denote them respectively by $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$ and $\underline{\Sigma}_{A_1} \times \cdots \times \underline{\Sigma}_{A_n}$. The reason to choose these definitions for the composition is that we do not have a simple description of spectra $f_1^*\underline{\Sigma}_{\underline{A_1}} \times ... \times f_n^*\underline{\Sigma}_{\underline{A_n}}$, while we have Eq. (5.18) for $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$.

Remark 24. The product on the right hand side of Eq. (5.19) does not change even if taken in the category of locales $\mathbf{Loc}_{[\prod_{i=1}^n \mathcal{C}(A_i),\mathbf{Sets}]}$ (not necessarily compact regular). This is because the product of compact regular locales (such as $\underline{\Sigma}_{f_i^*\underline{A_i}}$) in the category of locales is again compact and regular [96, 41], and because compact regular locales are automatically completely regular in $[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Sets}]$[7]. We need this property when constructing Markov chains in Chap. 6.

5.3 States on composite systems

The integrals over $\underline{A}$ ($A = \mathcal{B}(\mathcal{H})$) correspond bijectively to density operators on $\mathcal{H}$ [90]. This is an important evidence that the Bohrification approach describes quantum theory. This bijective correspondence is not generalised straightforwardly to composite systems. In the following, we show that integrals on composite systems corresponds to positive over pure tensor states (see Def. 5 for the definition of positive over pure tensor states).

[7]It is known that internal compact regular locales are completely regular if the topos in question satisfies the axiom of dependent choice [41], and every presheaf topos (including $[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Sets}]$) satisfies it [97]. This fact is already mentioned in Ref. [90]. Thus category $\mathbf{KRegLoc}_{[\prod_{i=1}^n \mathcal{C}(A_i),\mathbf{Sets}]}$ of compact regular locales internal to $[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Sets}]$ coincides with $\mathbf{KCRegLoc}_{[\prod_{i=1}^n \mathcal{C}(A_i),\mathbf{Sets}]}$.

5.3.1 Integrals over coproducts of algebras

Internal integrals over $\underline{A}$ in $[\mathcal{C}(A), \mathbf{Sets}]$ are natural transformations $I : \underline{A}_{sa} \to \mathbb{R}$ whose components $I_C : \underline{A}(C)_{sa} \to \mathbb{R}$ are all integrals in **Sets** [90]. We first extend this fact to integrals over $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$.

Theorem 25 (Integrals over $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$[95])**.** An integral over $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$ is a family $\{I_{(C_1,...,C_n)} : (C_1 \otimes ... \otimes C_n)_{sa} \to \mathbb{R}\}_{(C_1,...,C_n) \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n)}$ such that

1. each $I_{(C_1,...,C_n)} : (C_1 \otimes ... \otimes C_n)_{sa} \to \mathbb{R}$ is an integral in **Sets**, and
2. if $(C_1, ..., C_n) \leq (C'_1, ..., C'_n)$, then $I_{(C'_1,...,C'_n)}(a) = I_{(C_1,...,C_n)}(a)$ for all $a \in (C_1 \otimes ... \otimes C_n)_{sa}$.

Proof. See Appx. D.2. □

Integrals over $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$ correspond not to quantum states but to positive over pure tensor states.

Theorem 26. [95] There exists a bijective correspondence between positive over pure tensor states on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ and integrals over $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$, if the dimension of the Hilbert spaces $\mathcal{H}_i$ are all at least three. The integral $\{I^{\omega}_{(C_1,...,C_n)} : (C_1 \otimes ... \otimes C_n)_{sa} \to \mathbb{R}\}_{(C_1,...,C_n) \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n)}$ corresponding to a positive over pure tensor state ω is defined by

$$I^{\omega}_{(C_1,...,C_n)}(a) = \mathrm{Tr}\omega a, \tag{5.21}$$

for all $a \in (C_1 \otimes ... \otimes C_n)_{sa}$ and $(C_1, ..., C_n) \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n)$.

Proof. See Appx. D.3. □

The gap between density operators and integrals over composite systems is understandable from the observation that $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$ does not include contexts for entangled measurements. Consider a context $C_A \otimes C_B$ in the bipartite $\underline{A_1} \otimes \underline{A_2}$ with $A_1 \cong \mathcal{B}(\mathbb{C}_2)$ and $A_2 \cong \mathcal{B}(\mathbb{C}_2)$ for example. Marginal commutative C*-algebras C_A and C_B are generated by certain 1-dimensional projectors in $\mathbb{C}_2$ as

$$C_A = \{c_1|a_1\rangle\langle a_1| + c_2|a_2\rangle\langle a_2| \mid c_i \in \mathbb{C}\}, \tag{5.22}$$
$$C_B = \{c_1|b_1\rangle\langle b_1| + c_2|b_2\rangle\langle b_2| \mid c_i \in \mathbb{C}\}. \tag{5.23}$$

Then any operator O in $C_A \otimes C_B$ is decomposed uniquely to

$$\begin{aligned} O = \; & c_{11}|a_1\rangle\langle a_1| \otimes |b_1\rangle\langle b_1| + c_{12}|a_1\rangle\langle a_1| \otimes |b_2\rangle\langle b_2| \\ & + c_{21}|a_2\rangle\langle a_2| \otimes |b_1\rangle\langle b_1| + c_{22}|a_2\rangle\langle a_2| \otimes |b_2\rangle\langle b_2|. \end{aligned} \tag{5.24}$$

If we require O to be positive semi-definite, all the coefficients c_{ij} are non-negative. As a consequence, all the positive operators included in $C_A \otimes C_B$ are separable. Integrals over $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$ are required to be positive by the condition (5.9), but only for separable operators just like positive over pure tensor states.

Remark 27. Although Thm. 26 deals with the integrals over $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$ internal to topos $[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Set}]$, the same bijective correspondence exists between positive over pure tensor states in $\mathcal{W}(\mathcal{H}_1 \otimes ... \otimes \mathcal{H}_m)$ and integrals over $\underline{A_1} \otimes ... \otimes \underline{A_m}$ internal to $[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Set}]$ for any $m \leq n$. This is because integrals over $\underline{A_1} \otimes ... \otimes \underline{A_m} : (C_1, ..., C_n) \mapsto C_1 \otimes ... \otimes C_m$ in $[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Set}]$ $(m \leq n)$, and integrals over $\underline{A_1} \otimes ... \otimes \underline{A_m} : (C_1, ..., C_m) \mapsto C_1 \otimes ... \otimes C_m$ in $[\prod_{i=1}^m \mathcal{C}(A_i), \mathbf{Sets}]$ are equivalent.

5.3.2 Riesz theorem and valuations on products of spectra

From the constructive Riesz theorem, we have a locale isomorphism

$$\mathscr{V}(\underline{\Sigma}_{\underline{A_1} \otimes \cdots \otimes \underline{A_n}}) \cong \mathscr{I}(\underline{A_1} \otimes \cdots \otimes \underline{A_n}). \tag{5.25}$$

Isomorphisms (5.19) and (5.25) together imply

$$\mathscr{V}(\underline{\Sigma}_{A_1} \times \cdots \times \underline{\Sigma}_{A_n}) \cong \mathscr{I}(\underline{A_1} \otimes \cdots \otimes \underline{A_n}). \tag{5.26}$$

In words, the locales of integrals over the coproduct algebra and of valuations on the corresponding product spectra are isomorphic. The following corollary of Thm. 26 is lead by this observation.

Corollary 28. [95] There exists a bijective correspondence between positive over pure tensor states on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ and valuations on $\underline{\Sigma}_{A_1} \times \cdots \times \underline{\Sigma}_{A_n}$, if the dimension of the Hilbert spaces $\mathcal{H}_i$ are all at least three.

The isomorphism (5.26) provides a way to analyse states on composite systems from two viewpoints. In this section, we have used integrals over algebras, since they provide clearer expressions on the values they assign for observables. In the next chapter, we use valuations on spectra to define Markov chains and to analyse their property.

Now we see how the notion of complete positivity in topos quantum theory depends on the definition of composite systems. As Cor. 28 suggests, any positive over pure tensor states are regarded as states in topos quantum theory, if we define composite systems by $\underline{\Sigma}_{A_1} \times \cdots \times \underline{\Sigma}_{A_n}$. As we have reviewed in Sec. 2.1.1, if a positive map in quantum theory is applied on a part of bipartite quantum states, they are not necessarily transformed to quantum states. However, the resulting operators are regarded as states in topos quantum theory, since they are positive over pure tensor. Thus any positive quantum maps, if representable in a suitable way in topos quantum theory, are regarded also CP in topos quantum theory, if we define composite systems by $\underline{\Sigma}_{A_1} \times \cdots \times \underline{\Sigma}_{A_n}$. This is in the first place because the positivity of integrals (5.9) depends on the definition of C*-algebras for composite systems, and our C*-algebra $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$ does not contain the context for repelling non-positive positive over pure tensor states. If we had other definitions of composite systems where joint valuations correspond bijectively to quantum states, positive non-CP quantum maps should not be regarded as CP.

Although positive quantum maps are regarded as CP in our composite systems, it does not mean the maps in topos quantum theory have a bijective correspondence between positive quantum maps. Positive quantum maps may not find their representation in topos quantum theory, while quantum states are represented by valuations. First of all, we have not defined the maps in topos quantum theory yet. In the next chapter, we define maps in topos quantum theory as a direct generalisation of transition matrices, and analyse their properties. With these generalisations, it becomes possible to restate the relation between positive over pure tensor states and complete positivity in topos quantum theory in a more precise manner (see Sec. 6.2.1 for detail).

Remark 29. Although we have obtained a bijective correspondence between positive over pure tensor states and valuations (Cor. 28), we do not know the explicit description of the valuation themselves. This is partly because we did not obtain the explicit description of the product Gelfand spectrum, and also because it is difficult to interpret the bijective correspondence between integrals and valuations explicitly in out topos. In the next chapter, rather than trying to calculate the Gelfand spectrum explicitly, we employ a categorical analysis for Markov chains so that we can keep the abstract argument from Cor. 28.

Chapter 6

Markov chains for topos quantum theory

We have defined a composition of marginal systems for topos quantum theory, and analysed general states on composite systems in the previous chapter. This chapter is devoted to a specific class of states called Markov chains.

As we have seen in Sec. 1.3, classical Markov chains are those states generated by action of transition matrices. We regard this property as a definition of classical Markov chains, and generalise them to topos quantum theory. Kleisli morphisms of the *valuation monad* are used in the place of transition matrices, and thus these morphisms are regarded as maps (state transformations) in topos quantum theory. The Markov chains in topos quantum theory are expected to reflect properties of these morphisms. While we are motivated to see which of positive and CP maps appear as maps in topos quantum theory, our analysis on Markov chains rather indicates a triviality of maps.

We first give a definition of general Markov chains which does not rely on toposes but makes use of monads in Sec. 6.1. Several properties of Markov chains are derived solely from the conditions on monads. An introduction to valuation monad and its Kleisli category is given in Sec. 6.2. Finally, we define Markov chains in topos quantum theory with the valuation monad in Sec. 6.3. We analyse monogamy properties of positive over pure tensor states independently to topos theory, and apply it to analyse these Markov chains.

6.1 Markov chains for monads

The distribution monad for classical probability theory and the valuation monad for topos quantum theory are both commutative. In this section, we define Markov chains for general commutative monads on cartesian categories, and study their properties without relying on the specific monads in use. We find a condition shared by the distribution monad and the valuation monad, that leads the triviality of our Markov chain in topos quantum theory later in Sec. 6.3.

In order to define Markov chains, we formulate notions of "systems" and "states" in terms of monads and their Kleisli categories in Sec. 6.1.1. Based on these notions, we define Markov chains for strong monads over cartesian categories in Sec. 6.1.2. We also analyse the conditions on monads so that the defined Markov chains have similar properties to classical ones.

6.1.1 Notions of systems and states

Our motivation to consider monads comes from the observation that notions of joint distribution, marginal distribution and transition matrices are completely described by the distribution monad on **Sets** (see Sec. 1.3.5 for a review of distribution monad). The functor part of the distribution monad can be identified with

$$\text{system} \to \text{states},$$

assignment. Notions of systems, composite systems, states and joint states are required for defining Markov chains.

We first define "systems" as objects of a cartesian category $\mathbf{C}$ with product $\times : \mathbf{C}\times\mathbf{C} \to \mathbf{C}$ and the terminal object 1 (see Appx. C.2 for the monoidal structure of cartesian categories). Then the functor part $T : \mathbf{C} \to \mathbf{C}$ of a monad (T, η, μ) on $\mathbf{C}$ is assumed to assign state spaces for systems. States on X are morphisms from the terminal object $1 \to TX$ (equivalently, Kleisli morphisms $1 \to_{\mathcal{K}\ell} X$).

Composition of systems X and Y should be given by the product $X \times Y$, so that joint states are morphisms $1 \to T(X \times Y)$. We need canonical morphisms $T(X \times Y) \to TX$ and $T(X \times Y) \to TY$ to define marginal states (like partial trace in quantum theory). For the distribution monad, these canonical morphisms are defined by $\mathscr{D}\pi_X$ and $\mathscr{D}\pi_Y$, where $\pi_X : X \times Y \to X$ and $\pi_Y : X \times Y \to Y$ are projections for the cartesian product. In the following we assume that the canonical morphisms for marginals are given by projectors $T\pi$ for cartesian categories.

We further require the monad to be commutative with the unique Fubini map $i_{X,Y} : TX \times TY \to T(X \times Y)$ so that product states are well defined. Since the Fubini map $i_{X,Y} : \mathscr{D}X \times \mathscr{D}Y \to \mathscr{D}(X \times Y)$ of the distribution monad represents the construction of product states in $\mathscr{D}(X \times Y)$ from two marginal states in $\mathscr{D}X$ and $\mathscr{D}Y$, we straightforwardly extend it to define product states on $T(X \times Y)$ as those written by

$$i_{X,Y} \circ \langle p_X, p_Y \rangle, \tag{6.1}$$

with pairs of marginal states $p_X : 1 \to_{\mathcal{K}\ell} X$ and $p_Y : 1 \to_{\mathcal{K}\ell} Y$. If the monad (T, η, μ) were strong but not commutative, there would be two candidates for product states $\mathrm{dst} \circ \langle p_x, p_Y \rangle$ and $\mathrm{dst}' \circ \langle p_x, p_Y \rangle$ which are not necessarily equal.

6.1.2 Markov chains for commutative monads over cartesian categories

Now we define Markov chains for strong monads on cartesian categories, by straightforwardly generalising the classical ones presented by Eq. (1.45).

Definition 30. Let $\mathbf{C}$ be a cartesian category with the terminal object 1, and (T, η, μ) be a commutative monad with a Fubini map i defined by Eqs. (1.32) (and equivalently (1.33)). A joint state $m : 1 \to T(X_1 \times ... \times X_n)$ is said to be a Markov

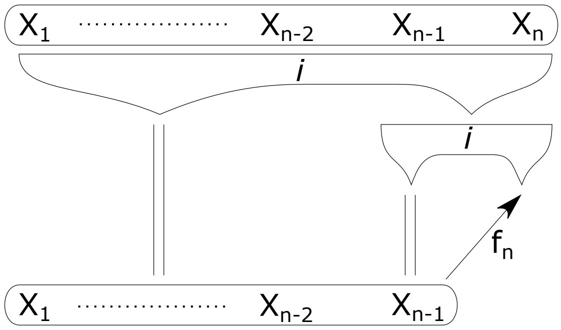

Figure 6.1: A configuration drawing of the process to extend Markov chains. Two equality represent the unit morphism η on the corresponding systems, and $f_n : X_{n-1} \to_{\mathcal{K}\ell} X_n$ represents the Kleisli morphism to extend the Markov chain. Boxes labelled by i denote the Fubini maps.

chain if there is a set of morphisms $\{f_i : X_{i-1} \to_{\mathcal{K}\ell} X_i\}_{i=1,\ldots,n}$ (with $X_0 := 1$) such that m is equal to

$$\mathrm{ext}_n \odot \mathrm{ext}_{n-1} \odot .... \odot \mathrm{ext}_3 \odot (i_{X_2,X_1} \circ \langle f_2, \eta_{X_1} \rangle) \odot f_1, \tag{6.2}$$

where

$$\mathrm{ext}_i \quad : \quad X_{i-1} \times ... \times X_1 \to_{\mathcal{K}\ell} X_i \times X_{i-1} \times ... \times X_1 \tag{6.3}$$

$$\mathrm{ext}_i \quad := \quad i_{X_i \times X_{i-1}, X_{i-2} \times ... \times X_1} \circ (i_{X_i, X_{i-1}} \circ \langle f_i, \eta_{X_i - 1} \rangle \times \eta_{X_{i-2} \times ... \times X_1}). \tag{6.4}$$

The morphisms ext_i "extend" Markov chains into larger Markov chains through the Kleisli morphism f_i (see Fig. 6.1 for a schematic representation). For the case of classical probability theory, this definition of Markov chains for distribution monad on **Sets** coincides with those of conventional definition presented by Eq. (1.23), or by Eq. (1.45) for the tripartite case. The transition matrices are generalised to Kleisli morphisms f_i.

While we have defined general Markov chains so that they coincide with the classical ones (1.23) if applied for probability distributions, the general ones may behave differently to the classical one. Here we consider several properties we expect for general Markov chains to have, and derive sufficient conditions on the monad to define these desirable Markov chains. Markov chains in topos quantum theory have these desirable properties since valuation monad is known to satisfy these sufficient conditions.

Stability of product states Let $p : 1 \to_{\mathcal{K}\ell} X \times Y$ be a bipartite state and $\mathrm{ext} : X \times Y \to_{\mathcal{K}\ell} X \times Y \times Z$ be defined by Eq. (6.8). If p is a product state then it would be natural to expect that $\mathrm{ext} \odot p$ is also a product state with regard to the bi-partition X and $Y \times Z$. Furthermore the marginal state on X should not be changed under the extension, since the extension map ext should be a local transformation on Y. In words, product states are expected to be stable under the extension. Product probability distributions are stable under the action of transition matrices.[1]

[1]Although trivial, any tripartite distribution defined by $p_{XYZ}(x, y, z) := f(y)(z)p_Y(y)p_X(x)$ with distributions p_X, p_Y and transition matrix f is again a product with respect to the bi-

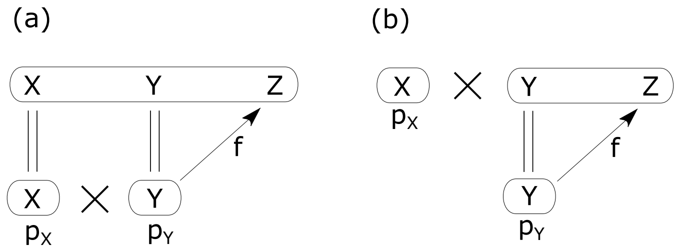

Figure 6.2: A schematic representation of Eq. (6.6). Equalities represent the unit morphism η on the corresponding systems, f is a Kleisli morphism. Symbols $\times$ are for product states. The left and right hand sides of Eq. (6.6) are expressed by (a) and (b), respectively.

The following lemma guarantees the stability of product states for any commutative monad.

Lemma 31. [95] Let (T, η, μ) be a commutative monad (T, η, μ) over cartesian category **C**. For all product state $i_{X,Y} \circ \langle p_X,\ p_Y \rangle : 1 \to_{\mathcal{K}\ell} X \times Y$ and all Kleisli morphisms $f : X \to_{\mathcal{K}\ell} X'$ and $g : Y \to_{\mathcal{K}\ell} Y'$, we have

$$(i_{X',Y'} \circ (f \times g)) \odot (i_{X,Y} \circ \langle p_X,\ p_Y \rangle) = i_{X',Y'} \circ \langle f \odot p_X, g \odot p_Y \rangle. \tag{6.5}$$

Proof. This lemma straightforwardly follows from the monoidal structure of i. See Appx. D.4 for an explicit proof. ☐

This lemma states that local transformations preserves product states if the monad is commutative. If applied to the extension ext, Lem. 31 suggests

$$\mathrm{ext} \odot \langle p_X, p_Y \rangle = i_{X,Y\times Z} \circ \langle p_X, (i_{Y,Z} \circ \langle \eta_Y, f \rangle) \odot p_Y \rangle, \tag{6.6}$$

where the right hand side represents a product state as desired. See Fig. 6.2 for a schematic representation of Eq. (6.6).

Locality of extension As we have seen in Sec. 1.3.3, a classical Markov chain has a property that the $n+1$-th random variable X_{n+1} depends on $X_{n-1},\ X_{n-2}, ...$ only through X_n. If we require this property for our Markov chain, we expect that the marginal state

$$T\pi_{Y\times Z} \circ (\mathrm{ext} \odot p), \tag{6.7}$$

$$(\mathrm{ext} := i_{X,Y\times Z} \circ (\eta_X \times i_{Y,Z} \circ \langle \eta_Y, f \rangle)) \tag{6.8}$$

with Kleisli morphisms $f : Y \to_{\mathcal{K}\ell} Z$ and $p : 1 \to_{\mathcal{K}\ell} X \times Y$, depends on p only through p's marginal on Y.

The following lemma suggests an explicit construction of the marginal state given by (6.7) from $T\pi_Y \circ p$.

Lemma 32. [95] Let $\mathrm{ext} : X \times Y \to_{\mathcal{K}\ell} X \times Y \times Z$ be defined as above by Eq. (6.8). The marginal state given by (6.7) satisfies

$$T\pi_{Y\times Z} \circ (\mathrm{ext} \odot p) = (i_{Y,Z} \circ \langle \eta_Y, f \rangle) \odot (T\pi_Y \circ p). \tag{6.9}$$

for any state $p : 1 \to_{\mathcal{K}\ell} X \times Y$.

partition X-YZ.

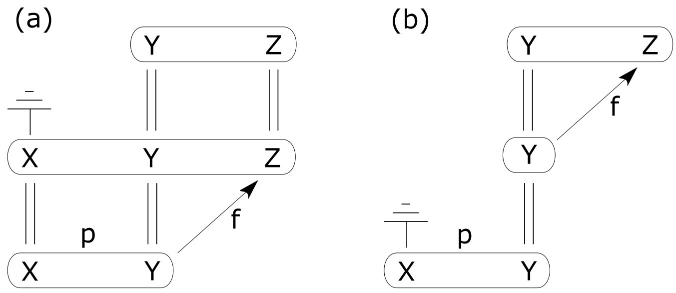

Figure 6.3: A schematic representation of Eq. (6.9). Equalities represent the unit morphism η on the corresponding systems and f is a Kleisli morphism. The systems with ground symbols are discarded to take the marginal states on the other parts. The left and right hand sides of Eq. (6.9) are expressed by (a) and (b), respectively.

Proof. See Appx. D.5. □

The right-hand-side of Eq. (6.9) reveals that $T\pi_{Y\times Z} \circ (\mathrm{ext} \odot p)$ depends on p only through its marginal on Y.[2] See Fig. 6.3 for a schematic representation of Eq. (6.9).

Preservation of original states While the morphism ext_i presented by Eq. (6.4) extends Markov chains, it might change the original state after extension. More precisely, we are not sure if

$$T\pi_{X\times Y} \circ (\mathrm{ext} \odot p) = p \tag{6.11}$$

$$(\mathrm{ext} := i_{X,Y\times Z} \circ (\eta_X \times i_{Y,Z} \circ \langle \eta_Y, f\rangle)) \tag{6.12}$$

holds for any Kleisli morphisms $f : Y \to_{\mathcal{K}\ell} Z$ and $p : 1 \to_{\mathcal{K}\ell} X \times Y$, and any set of systems $\{X,\ Y,\ Z\}$. See Fig. 6.4 for a schematic representation of the desired property (6.11). We already know that this is satisfied for the distribution monad[3].

We derive a sufficient condition on monad (T, η, μ) to satisfy Eq. (6.11) for any Markov chains.

Lemma 33. [95] Equation (6.11) holds if $T1 \cong 1$.

Proof. See Appx. D.6. □

In summary, the stability of product states under extension (6.6) is guaranteed and the marginal of extended states coincides with the extension of marginal

[2]For the distribution monad, Eq. (6.9) comes down to an almost trivial equation

$$\sum_{x\in X} p(x,y)f(y)(z) = f(y)(z)\sum_{x\in X} p(x,y). \tag{6.10}$$

[3]If $p : X \times Y \to [0,1]$ is a joint distribution and $[f(y)(z)]_{y,z}$ is a transition matrix from Y to Z, Eq. (6.11) reduces to

$$\sum_{z\in Z} p(x,y)f(y)(z) = p(x,y), \tag{6.13}$$

which is obvious from $\sum_{z\in Z} f(y)(z) = 1$.

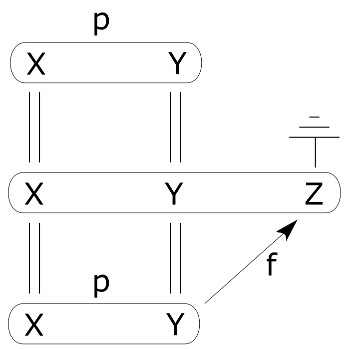

Figure 6.4: A schematic representation of Eq. (6.11). Equalities represent the unit morphism η on the corresponding systems, f is a Kleisli morphism, and the marginal onto systems without the ground symbol is taken.

states (namely, Eq. (6.9) holds) in any commutative monad over cartesian categories. Extensions preserve original states (namely, Eq. (6.11) holds) if $T1 \cong 1$. We have obtained these results without relying on explicit descriptions of commutative monads and Kleisli morphisms therein. These results find their uses in the next section, where we do not have explicit description of Kleisli morphisms of the valuation monad.

Remark 34. The distribution monad has

$$\mathscr{D}1 = \{p : \{*\} \to [0,1] \mid p(*) = 1\} = \{\delta_*\} \cong 1. \tag{6.14}$$

There are many examples of commutative monads with $T1 \cong 1$ other than the distribution monad: Giry monad on measurable spaces [63], Radon monad on compact Hausdorff spaces [60], and the valuation monad on locales. These examples are all somehow related to probability weight functions, where $\mathscr{D}1 \cong 1$ states the normalisation of weight functions just as Eq. (6.14) does.

Remark 35. There are commutative monads which do not have $T1 \cong 1$ but still validate Eq. (6.11). An example which may be related to quantum physics is the Fock space monad $\mathcal{F}$ presented in Ref. [98].

Remark 36. The extension of the bipartite distribution ext $\odot$ p represents a solution of the "extension problem" for classical probability distributions. The extension problem asks for necessary and sufficient conditions for a pair of bipartite states p_{XY} on $X \times Y$ and p_{YZ} on $Y \times Z$ to be expressed as marginal states of a tripartite state p_{XYZ} (called an extension of p_{XY} and p_{YZ}). It is known that if p_{XY} and p_{YZ} are probability distributions, their extension probability distribution p_{XYZ} exists if and only if they coincides on the common marginal Y [99]. An extension can be constructed by

$$p_{XYZ}(x, y, z) := p_{Z|Y}(y)(z)p_{XY}(x, y), \tag{6.15}$$

where $p_{Z|Y}$ is the conditional distribution $p_{Z|Y}(y)(z) := p_{YZ}(y, z)/p_Y(y)$ regarded as a transition matrix. This extension is equal to ext $\odot$ p if we substitute p_{XY} to p, and $p_{Z|Y}$ to f inside ext.

6.2 Kleisli morphisms of valuation monad

Here, we give an introduction to valuation monad and its Kleisli category. We review a relation between Kleisli morphisms of valuation monad and transition matrices, which motivate us to use the former as maps in topos quantum theory. We also include a review on other related monads recently studied in Rem. 37. Subsection 6.2.1 summarises our observation between the relation of complete positivity and commutativity of monads.

Valuation monad is a monad on category of locales **Loc** presented in Ref. [100].[4] The functor part $\mathscr{V} : \mathbf{Loc} \to \mathbf{Loc}$ assigns the locale of valuations $\mathscr{V}X$ for a given locale X. If X is a compact, completely regular locale, $\mathscr{V}X$ coincides with the one presented in Ref. [49] and reviewed in Sec. 5.1.1. The valuation monad is commutative much like the distribution monad.

Kleisli morphisms of the valuation monad include transition matrices of classical probability theory as a special case. If both of locales X and Y internal to **Sets** are a finite set with discrete topology, Kleisli morphisms $X \to \mathscr{V}Y$ are the same things to Kleisli morphisms $X \to \mathscr{D}Y$ of the distribution monad, that is, transition matrices. Thus they naturally generalise transition matrices to topos quantum theory.

As we have reviewed in Sec. 5.1.1, valuations on X have bijective correspondence between $\mathrm{Hom}_{\mathbf{Loc}}(1, X)$ where 1 is the terminal object in **Loc**. In other words, a valuation v on locale X is equivalent to a Kleisli morphism $v : 1 \to_{\mathcal{K}\ell} X$ of the valuation monad, in the same way probability distribution p on random variable X is equivalent to a Kleisli morphism $p : 1 \to_{\mathcal{K}\ell} X$ of the distribution monad (see Sec.1.3.5). The action of Kleisli morphism $f : X \to_{\mathcal{K}\ell} Y$ of the valuation monad on the valuation v is defined by the Kleisli composition

$$f \odot v : 1 \xrightarrow{v} \mathscr{V}X \xrightarrow{\mathscr{V}f} \mathscr{V}^2 Y \xrightarrow{\mu_Y} \mathscr{V}Y \tag{6.16}$$

in exactly the same way transition matrices acts on probability distributions. Once a composition of transition matrices is written by Kleisli morphisms, its valuation version is immediately obtained by replacing the monad to valuations. This property is useful when we generalise concepts such as Markov chains from classical probability theory to topos quantum theory.

Remark 37. Recent studies from computer science reinforce connections between positive and CP maps of C*-algebras and Kleisli morphisms. As we have reviewed in Sec. 1.3.2, positive (=CP) maps on finite dimensional commutative C*-algebras have bijective correspondence between transition matrices. This is revealed by the equivalence

$$\mathbf{FdcCstar}^{op}_{\mathrm{PU}} \cong \mathcal{K}\ell_{\mathbb{N}}(\mathscr{D}) \tag{6.17}$$

of category $\mathbf{FdcCstar}^{op}_{\mathrm{PU}}$ of finite dimensional commutative C*-algebras and unital positive maps, and Kleisli category $\mathcal{K}\ell_{\mathbb{N}}(\mathscr{D})$ of the distribution monad with a restriction on the underlying category [60]. In words, the distribution monad provides a (non-trivial) Kleisli representation of $\mathbf{FdcCstar}^{op}_{\mathrm{PU}}$. Table 6.1 summarises

[4]Vickers presents three types of valuation monads, representing unnormalised, subnormalised, and normalised valuations, respectively [100]. In this thesis, we focus only on valuation monad for normalised valuations.

other categories of C*-algebras whose Kleisli representations are found. It is still

Category	C*-algebras	morphism	Kleisli representation
$\mathbf{cCstar}^{op}_{\mathrm{PU}}$	commutative	unital positive	$\mathcal{K}\ell(\mathcal{R})$ ([60])
$\mathbf{Cstar}^{op}_{PU}$	noncommutative	unital positive	[101]
$\mathbf{Cstar}^{op}_{CPU}$	noncommutative	unital CP	[101]

Table 6.1: Categories of C*-algebras and their corresponding Kleisli representations. The second and third columns show the sorts of C*-algebra objects and morphisms of the categories in the first column, respectively. The fourth column presents the corresponding Kleisli category and the corresponding references. The functor part $\mathcal{R} : \mathbf{KHausSp} \to \mathbf{KHausSp}$ of the Radom monad assigns Radom measures on compact Hausdorff spaces [60]. It is shown that there exists Kleisli representation for $\mathbf{Cstar}^{op}_{PU}$ and $\mathbf{Cstar}^{op}_{CPU}$ in Ref. [101], while their explicit expression are still unknown. All the categories are internal to **Sets**.

not known if the Kleisli category of valuation monad represents certain category of C*-algebras. Thus we still do not know if its Kleisli morphisms corresponds to internal maps on C*-algebras.

6.2.1 Spatial composition of Kleisli morphisms

Temporal composition of two Kleisli morphisms are defined by the Kleisli composition. The unique Fubini map on commutative monad defines spatial composition of Kleilsi morphisms acting in parallel. Here we observe that all Kleisli morphisms are guaranteed to be CP in a certain sense if their spatial composition is defined by the Fubini map.

Let (T, η, μ) be a commutative monad over a cartesian category $\mathbf{C}$, i be its Fubini map, and $f : X \to_{\mathcal{K}\ell} X'$ and $g : Y \to_{\mathcal{K}\ell} Y'$ be Kleisli morphisms. The *spatial composition* of f and g refers to a Kleisli morphism $f \otimes g : X \times Y \to_{\mathcal{K}\ell} X' \times Y'$ defined by

$$f \otimes g := i_{X',Y'} \circ (f \times g). \tag{6.18}$$

For readers with familiarity on category theory, it suffices to say that Kleisli categories of commutative monads have monoidal structure $\otimes$ [102].

All the Kleisli morphisms of a commutative monad is completely positive in the sense that arbitrary spatial composition of two Kleisli morphisms are allowed. CP maps in quantum and classical probability theories are defined to send states to (possibly unnormalised) states, if it act in parallel with identity maps. If we define the states on system $X \times Y$ to be Kleisli morphisms $v : 1 \to_{\mathcal{K}\ell} X \times Y$, the parallel action of the Kleisli morphism $f : X \to_{\mathcal{K}\ell} X'$ and the identity on Y transforms it to

$$(f \otimes \eta_Y) \odot v, \tag{6.19}$$

which is a state on $X' \times Y$ (note that unit η_Y is the identity morphism on Y in the Kleisli category). Thus any Kleisli morphisms are valid state transformation even if they acts on marginal systems.

We shall restate our comment on the relationship between positive over pure tensor states and complete positivity in topos quantum theory presented in Sec. 5.3.2

more precisely. With regard to our composite system in topos quantum theory, valuations on $\underline{\Sigma}_{A_1} \times \underline{\Sigma}_{A_2}$ bijectively corresponds to positive over pure tensor states on $\mathcal{H}_1 \otimes \mathcal{H}_2$, if $A_1 = \mathcal{B}(\mathcal{H}_1)$ and $A_2 = \mathcal{B}(\mathcal{H}_2)$. Let $v : 1 \to_{\mathcal{K}\ell} \underline{\Sigma}_{A_1} \times \underline{\Sigma}_{A_2}$ be a valuation, and $f : \underline{\Sigma}_{A_1} \to_{\mathcal{K}\ell} \underline{\Sigma}_{A_1}$ be a Kleisli morphism of the valuation monad. Then a valuation

$$v' := (f \otimes \eta_{\underline{\Sigma}_{A_2}}) \odot v \tag{6.20}$$

corresponds not necessarily to a quantum state, but to a positive over pure tensor state on $\mathcal{H}_1 \otimes \mathcal{H}_2$. Thus even if f corresponds to a positive non-CP map in quantum theory and v' does not corresponds to a quantum state, it is regarded to be CP in our definition of composite systems in topos quantum theory. If there is another definition of composite systems that leads to a bijective correspondence between joint valuations and quantum states, Kleisli morphisms do not represent positive non-CP maps in quantum theory.

Nevertheless the above argument does not indicate the existence of Kleisli morphisms corresponding to positive maps. It only denies the existence of Kleisli morphisms corresponding to non-positive maps. More work is required to see which of the positive and CP maps in quantum theory, topos quantum theory leads when generalising classical probability theory.

6.3 Valuation monad for topos quantum theory

This section applies results from Sec. 6.1 to the topos quantum systems of Chap. 5, by considering the valuation monad on the category of locales **Loc** internal to toposes. Category **Loc** is cartesian [103], and the valuation monad is commutative and satisfies $\mathscr{V}1 \cong 1$ [100], making this application possible.

Before going to Markov chains in topos quantum theory, we analyse properties of positive over pure tensor states in Sec. 6.3.1. We show that monogamy of multipartite quantum states, which is a characteristic property of quantum states that classical probability does not have, also exists for positive over pure tensor states. From the monogamy of positive over pure tensor states, we deduce that every Markov chain of the valuation monad for topos quantum theory must be a product state in Sec. 6.3.2. Thus we show a triviality of Markov chains.

6.3.1 Monogamy of positive over pure tensor states

In this subsection, we check that a monogamy property of quantum states also holds for positive over pure tensor states. The results of this subsection is combined with those of Sec. 6.1.2 to prove the triviality of Markov chains in topos quantum theory.

Monogamy in quantum theory means the following property of quantum correlations, namely, if a tripartite state has a strong correlation in one of its bipartite marginal system, then the marginal system does not have a strong correlation between the third. This property of quantum correlations partly originates from non-trivial *extendibility* conditions of marginal quantum states, which are considered in quantum marginal problems. Among many extendibility situations, we focus on the simplest one by replacing quantum states into positive over pure tensor states. We denote the set of positive over pure tensor states on composite system $\mathcal{H}_X \otimes \mathcal{H}_Y \otimes ...$ by $\mathcal{W}(\mathcal{H}_X \otimes \mathcal{H}_Y \otimes ...)$.

Definition 38. A pair of bipartite positive over pure tensor states $\omega_{XY} \in \mathcal{W}(\mathcal{H}_X \otimes \mathcal{H}_Y)$ and $\omega_{YZ} \in \mathcal{W}(\mathcal{H}_Y \otimes \mathcal{H}_Z)$, is said to be *extendible* if there exists a tripartite positive over pure tensor state $\omega_{XYZ} \in \mathcal{W}(\mathcal{H}_X \otimes \mathcal{H}_Y \otimes \mathcal{H}_Z)$ such that

$$\mathrm{Tr}_{\mathcal{H}_X}[\omega_{XYZ}] = \omega_{YZ}, \tag{6.21}$$

$$\mathrm{Tr}_{\mathcal{H}_Z}[\omega_{XYZ}] = \omega_{XY}. \tag{6.22}$$

An obvious necessary condition for a pair $(\omega_{XY}, \omega_{YZ})$ to be extendible is $\mathrm{Tr}_{\mathcal{H}_X}[\omega_{XY}] = \mathrm{Tr}_{\mathcal{H}_Z}[\omega_{YZ}]$, namely, they must coincide on the overlapping marginal.

The analogous concept of extendibility can be defined for classical probability distributions and quantum states as well [99]. As we have remarked in Rem. 36, any pair of classical probability distributions with marginal states coinciding on the overlap is extendible. This is not the case for quantum states (see e.g. [99, 104]), and positive over pure tensor states as we will see below.

As we have seen in Sec. 2.1.1, the set of bipartite positive over pure tensor states is convex whose extremal points of which can be characterised [66]. Examples of extremal bipartite positive over pure tensor states are pure quantum states, and partial transpositions of those.

Lemma 39. [95] Let $\mathcal{H}_X,\ \mathcal{H}_Y,\ \mathcal{H}_Z$ be Hilbert spaces, and $\omega \in \mathcal{W}(\mathcal{H}_X \otimes \mathcal{H}_Y \otimes \mathcal{H}_Z)$ be a positive over pure tensor state. If $\mathrm{Tr}_{\mathcal{H}_Z}(\omega)$ is an extremal bipartite positive over pure tensor state[5] on $\mathcal{H}_Y \otimes \mathcal{H}_Z$, then $\omega = \mathrm{Tr}_{\mathcal{H}_Z}(\omega) \otimes \mathrm{Tr}_{\mathcal{H}_X \otimes \mathcal{H}_Y}(\omega)$.

Proof. If $\{O_i \in \mathcal{B}(\mathcal{H}_Z)\}_{i=1,\dots,m}$ is a set of POVM measurement operators, then operators on $\mathcal{H}_X \otimes \mathcal{H}_Y$ defined by

$$\omega|_i := \mathrm{Tr}_{\mathcal{H}_Z}[\omega(\mathbb{I}_{\mathcal{H}_X \otimes \mathcal{H}_Y} \otimes O_i)]/p_i, \tag{6.23}$$

$$(p_i := \mathrm{Tr}[\omega(\mathbb{I}_{\mathcal{H}_X \otimes \mathcal{H}_Y} \otimes O_i)] = \mathrm{Tr}\left[\mathrm{Tr}_{\mathcal{H}_X \otimes \mathcal{H}_Y}[\omega] O_i\right] \geq 0) \tag{6.24}$$

are positive over pure tensor states on $H_1 \otimes H_2$, since

$$\mathrm{Tr}[\omega|_i] = \frac{\mathrm{Tr}[\omega(\mathbb{I}_{\mathcal{H}_X \otimes \mathcal{H}_Y} \otimes O_i)]}{\mathrm{Tr}[\omega(\mathbb{I}_{\mathcal{H}_X \otimes \mathcal{H}_Y} \otimes O_i)]} = 1, \text{ and} \tag{6.25}$$

$$\mathrm{Tr}[\omega|_i(P_X \otimes P_Y)] = \mathrm{Tr}_{\mathcal{H}_Z}[\omega(P_X \otimes P_Y \otimes O_i)]/p_i \geq 0, \tag{6.26}$$

hold for any positive operators P_X and P_Y on $\mathcal{H}_X$ and $\mathcal{H}_Y$. The marginal state is represented by a convex combination of positive over pure tensor states

$$\mathrm{Tr}_{\mathcal{H}_Z}[\omega] = \mathrm{Tr}_{\mathcal{H}_Z}[\omega(\mathbb{I}_{\mathcal{H}_X \otimes \mathcal{H}_Y} \otimes \sum_{i=1}^{m} O_i)] = \sum_i p_i \omega|_i, \tag{6.27}$$

[5]Note that if $\omega \in \mathcal{W}(\mathcal{H}_X \otimes \mathcal{H}_Y \otimes ...)$ is a positive over pure tensor state, its partial traces $\mathrm{Tr}_{\mathcal{H}_i}[\omega]$ are positive over pure tensor states.

Since $\mathrm{Tr}_{\mathcal{H}_Z}[\omega]$ is assumed to be an extremal bipartite state, it follows that the states $\omega|_i$ are all equal to $\mathrm{Tr}_{\mathcal{H}_Z}[\omega]$. Then for any set of positive operators $\{P_X,\ P_Y,\ P_Z\}$ $(P_i \in \mathcal{H}_i)$,

$$\begin{aligned}\mathrm{Tr}[\omega(P_X \otimes P_Y \otimes P_Z)] &= \mathrm{Tr}\left[(P_X \otimes P_Y)\mathrm{Tr}_{\mathcal{H}_Z}[\omega(\mathbb{I}_{\mathcal{H}_X\otimes\mathcal{H}_Y} \otimes P_Z)]\right] \\ &= \mathrm{Tr}\left[(P_X \otimes P_Y)\mathrm{Tr}_{\mathcal{H}_Z}[\omega]\right] \times \mathrm{Tr}\left[P_Z \mathrm{Tr}_{\mathcal{H}_X\otimes\mathcal{H}_Y}[\omega]\right] \\ &= \mathrm{Tr}\left[(P_X \otimes P_Y \otimes P_Z)\left(\mathrm{Tr}_{\mathcal{H}_Z}[\omega] \otimes \mathrm{Tr}_{\mathcal{H}_X\otimes\mathcal{H}_Y}[\omega]\right)\right]\end{aligned}$$

holds. This implies $\omega = \mathrm{Tr}_{\mathcal{H}_Z}[\omega] \otimes \mathrm{Tr}_{\mathcal{H}_X\otimes\mathcal{H}_Y}[\omega]$ as claimed in the lemma. □

Lemma 40. [95] If either of a pair of nonproduct positive over pure tensor states $\omega_{XY} \in \mathcal{W}(\mathcal{H}_X \otimes \mathcal{H}_Y)$ or $\omega_{YZ} \in \mathcal{W}(\mathcal{H}_Y \otimes \mathcal{H}_Z)$ is extremal, the pair is not extendible.

Proof. Without loss of generality we assume that ω_{XY} is an extremal nonproduct positive over pure tensor state. If there is a tripartite state ω_{XYZ} with the property presented in the lemma, it follows from the previous lemma that ω_{XYZ} is expressed as $\omega_{XYZ} = \omega_{XY} \otimes \mathrm{Tr}_{\mathcal{H}_X\otimes\mathcal{H}_Y}(\omega_{XYZ})$. Then $\mathrm{Tr}_{\mathcal{H}_X}[\omega_{XYZ}]$ is a product state, contradicting to the assumption that ω_{YZ} is a nonproduct state. □

Note that bipartite positive over pure tensor states which are simultaneously non-product and extremal do exist. Examples are the non-product pure quantum states and their partial transpositions.

These lemmas can be interpreted as evidences of the monogamy of positive over pure tensor states. A pair of bipartite positive over pure tensor states ω_{XY} and ω_{YZ} is not necessarily extendible even if they coincide on the overlap $\mathcal{H}_Y$. There are non-trivial extendibility conditions beyond the coincidence on overlaps, and this condition prohibits multipartite quantum states to have arbitrary strong correlations in all partitioning. In particular, Lem. 39 reveals that if a bipartite marginal state on a tripartite positive over pure tensor state is extremal, then the tripartite state must be a product of the bipartite marginal state and the rest.

We further analyse details of this monogamy property for showing a triviality of Markov chains in the next section.

Theorem 41. [95] For any non-product positive over pure tensor state ω_{XY} on $\mathcal{H}_X \otimes \mathcal{H}_Y$, there is a quantum state ρ_{YZ} on $\mathcal{H}_Y \otimes \mathcal{H}_Z$ with $\dim \mathcal{H}_Z = 3$ such that $\mathrm{Tr}_{\mathcal{H}_X}[\omega_{XY}] = \mathrm{Tr}_{\mathcal{H}_Z}[\rho_{YZ}]$ but the pair (ω_{XY}, ρ_{YZ}) is not extendible.

Proof. Denote the marginal state on $\mathcal{H}_Y$ by $\rho_Y := \mathrm{Tr}_{\mathcal{H}_X}[\omega_{XY}]$. Define rank-2 projectors Π_{ij} $(i, j = 1, ..., \dim \mathcal{H}_Y,\ i \neq j)$ by

$$\Pi_{ij} = |\psi_i\rangle\langle\psi_i| + |\psi_j\rangle\langle\psi_j|, \tag{6.28}$$

where $\{|\psi_i\rangle\}_{i=1,...,\dim \mathcal{H}_Y}$ is the basis diagonalising ρ_Y so that $\rho_Y = \sum_i p_i |\psi_i\rangle\langle\psi_i|$.

We first show that if ω_{XY} is not a product state, there exists a pair $i, j \in \{1, ..., \dim \mathcal{H}_Y\}$ such that

$$(\mathbb{I}_{\mathcal{H}_X} \otimes \Pi_{ij})\omega_{XY}(\mathbb{I}_{\mathcal{H}_X} \otimes \Pi_{ij}) \tag{6.29}$$

is not product. If we assume the contrary,

$$(\mathbb{I}_{\mathcal{H}_X} \otimes \Pi_{ij})\omega_{XY}(\mathbb{I}_{\mathcal{H}_X} \otimes \Pi_{ij}) = O_{ij}^{\mathcal{H}_X} \otimes O_{ij}^{\mathcal{H}_Y} \tag{6.30}$$

holds for all pairs $i \neq j$. Then for any one dimensional projector,

$$\begin{aligned}
& (\mathbb{I}_{\mathcal{H}_X} \otimes |\psi_i\rangle\langle\psi_i|)\omega_{XY}(\mathbb{I}_{\mathcal{H}_X} \otimes |\psi_i\rangle\langle\psi_i|) \\
= \; & (\mathbb{I}_{\mathcal{H}_X} \otimes |\psi_i\rangle\langle\psi_i|\Pi_{ij})\omega_{XY}(\mathbb{I}_{\mathcal{H}_X} \otimes \Pi_{ij}|\psi_i\rangle\langle\psi_i|) \\
\propto \; & O^{\mathcal{H}_X}_{ij} \otimes |\psi_i\rangle\langle\psi_i|.
\end{aligned} \tag{6.31}$$

Since this holds for any j not equal to i, we obtain $O^{\mathcal{H}_X}_{ij} \propto O^{\mathcal{H}_X}_{ij'}$ for any pair $j, j'(\neq i)$. Since $O^{\mathcal{H}_X}_{ij}$ is not changed under the permutation of i and j, there exists an operator $O^{\mathcal{H}_X}$ on $\mathcal{H}_X$ such that

$$O^{\mathcal{H}_X} \propto O^{\mathcal{H}_X}_{ij}, \tag{6.32}$$

for any $i \neq j$. This implies

$$\begin{aligned}
& \omega_{XY} \\
= \; & \sum_{i \neq j}(\mathbb{I}_{\mathcal{H}_X} \otimes \Pi_{ij})\omega_{XY}(\mathbb{I}_{\mathcal{H}_X} \otimes \Pi_{ij}) - \sum_k (\mathbb{I}_{\mathcal{H}_X} \otimes |\psi_k\rangle\langle\psi_k|)\omega_{XY}(\mathbb{I}_{\mathcal{H}_X} \otimes |\psi_k\rangle\langle\psi_k|) \\
\propto \; & O^{\mathcal{H}_X} \otimes O^{\mathcal{H}_Y},
\end{aligned}$$

with an operator $O^{\mathcal{H}_Y}$ on $\mathcal{H}_Y$, which contradicts to the assumption that ω_{XY} is not product.

Without loss of generality, we assume that the case of $i = 1, j = 2$ gives a non-product operator by Eq. (6.29). Define $|\phi\rangle_{23}$ as an unnormalised purification of $p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|$

$$|\phi\rangle_{YZ} := \sqrt{p_1}|\psi_1\rangle \otimes |0\rangle_Z + \sqrt{p_2}|\psi_2\rangle \otimes |1\rangle_Z, \tag{6.33}$$

and define ρ_{YZ} by

$$\rho_{YZ} := |\phi\rangle\langle\phi|_{YZ} + \sum_{i \geq 3} p_i|\psi_i\rangle\langle\psi_i| \otimes |2\rangle\langle 2|_Z, \tag{6.34}$$

so that the marginal state $\mathrm{Tr}_{\mathcal{H}_Z}[\rho_{YZ}]$ on $\mathcal{H}_Y$ is equal to ρ_Y.

ρ_{YZ} is not extendible with ω_{XY}. Otherwise there exists a tripartite positive over pure tensor state ω_{XYZ} whose marginals are ω_{XY} and ρ_{YZ}. The restriction of ω_{XYZ}

$$(\mathbb{I}_{\mathcal{H}_X} \otimes \Pi_{12} \otimes \mathbb{I}_{\mathcal{H}_Z})\omega_{XYZ}(\mathbb{I}_{\mathcal{H}_X} \otimes \Pi_{12} \otimes \mathbb{I}_{\mathcal{H}_Z}), \tag{6.35}$$

must have marginals $(\mathbb{I}_{\mathcal{H}_X} \otimes \Pi_{12})\omega_{XY}(\mathbb{I}_{\mathcal{H}_X} \otimes \Pi_{12})$ and $|\phi\rangle\langle\phi|_{YZ}$. This contradicts to Lem. 40 since both of them are non-product and $|\phi\rangle\langle\phi|_{YZ}$ is (proportional to) a pure state, which is an extremal point of $\mathcal{W}(\mathcal{H}_Y \otimes \mathcal{H}_Z)$. □

6.3.2 Triviality of Markov chains

We denote the Fubini map of valuation monad by $i_{X,Y} : \mathscr{V}X \times \mathscr{V}Y \to \mathscr{V}(X \times Y)$. Similarly to the Fubini map for distribution monad, i represents inclusion of product valuations to the space (locale, in precise) of valuations on composite system [100]. Product valuations on $X \times Y$ are those defined by

$$i \circ \langle v_X, v_Y\rangle : 1 \to_{\mathcal{K}\ell} X \times Y \tag{6.36}$$

with valuations $v_X : 1 \to_{\mathcal{K}\ell} X$ and $v_Y : 1 \to_{\mathcal{K}\ell} Y$ on local systems X and Y, respectively.

Now consider the valuation monad on the category of locales internal to the topos $[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Sets}]$, where $A_i = \mathcal{B}(\mathcal{H}_i)$ are non-commutative algebras of operators on finite dimensional Hilbert spaces. Valuations on $\prod_{i\in I} \underline{\Sigma}_{A_i}$, where I is a subset of $\{1, ..., n\}$, correspond to positive over pure tensor states on $\bigotimes_{i\in I} \mathcal{H}_i$ by Thm. 26. Product valuations correspond to product quantum states. Taking marginals of a valuation is equivalent to taking partial traces of the corresponding positive over pure tensor state.

Theorem 42. [95] Let $\mathcal{H}_i$ $(i = 1, ..., n)$ be finite dimensional Hilbert spaces all with dimensions at least 3. Markov chains of valuations on $\underline{\Sigma}_{A_1} \times \cdots \times \underline{\Sigma}_{A_n}$ defined by Def. 30, are equivalent to product states by the bijective correspondence (5.21).

Proof. Let $f_i : \underline{\Sigma}_{A_{i-1}} \to_{\mathcal{K}\ell} \underline{\Sigma}_{A_i}$ be Kleisli morphisms where $\underline{\Sigma}_{A_0} := 1$ for the terminal object 1 of $\mathbf{Loc}_{[\prod_{i=1}^n \mathcal{C}(A_i), \mathbf{Set}]}$. A sequence of Markov chains $v_i : 1 \to_{\mathcal{K}\ell} \underline{\Sigma}_{A_1} \times ... \times \underline{\Sigma}_{A_i}$ are constructed by

$$v_i := \mathrm{ext}_i \odot \mathrm{ext}_{i-1} \odot ... \odot \mathrm{ext}_3 \odot (i_{\underline{\Sigma}_{A_1}, \underline{\Sigma}_{A_2}} \circ \langle \eta_{\underline{\Sigma}_{A_1}}, f_2 \rangle) \odot f_1, \tag{6.37}$$

where

$$\mathrm{ext}_i := i_{\underline{\Sigma}_{A_1} \times ... \times \underline{\Sigma}_{A_{i-2}}, \underline{\Sigma}_{A_{i-1}} \times \underline{\Sigma}_{A_i}} \circ (i_{\underline{\Sigma}_{A_{i-1}}, \underline{\Sigma}_{A_i}} \circ \langle f_i, \eta_{\underline{\Sigma}_{A_{i-1}}} \rangle \times \eta_{\underline{\Sigma}_{A_1} \times ... \times \underline{\Sigma}_{A_{i-2}}}). \tag{6.38}$$

We inductively show that the Markov chains v_i presented in Eq. (6.37) are product valuations and hence corresponds to product quantum states.

We first deduce a contradiction by assuming the top one of this sequence

$$v_2 = (i_{\underline{\Sigma}_{A_1}, \underline{\Sigma}_{A_2}} \circ \langle \eta_{\underline{\Sigma}_{A_1}}, f_2 \rangle) \odot f_1 \tag{6.39}$$

corresponds to non-product positive over pure tensor states. We denote the quantum state corresponding to v_2 by ρ_2. If ρ_2 is not a product state, then v_2's marginal $\mathscr{V}\pi_{\underline{\Sigma}_{A_1}} \circ v_2$ corresponds to a mixed quantum state $\mathrm{Tr}_{\mathcal{H}_2}[\rho_2]$. Lemma 41 implies that there exists a valuation v_2' on system $\underline{\Sigma}_{A_1} \times \underline{\Sigma}_{A_3} \times ... \times \underline{\Sigma}_{A_n}$ corresponding to a quantum state ρ_2' whose marginal on $\mathcal{H}_1$ is equivalent to $\mathrm{Tr}_{\mathcal{H}_2}[\rho_2]$, but ρ_2 and ρ_2' are not marginal states of a single tripartite state. Now consider a valuation v on $\underline{\Sigma}_{A_1} \times \cdots \times \underline{\Sigma}_{A_n}$ defined by

$$v := \Big(i_{\underline{\Sigma}_{A_1} \times \underline{\Sigma}_{A_2}, \underline{\Sigma}_{A_3} \times ... \times \underline{\Sigma}_{A_n}} \circ (i_{\underline{\Sigma}_{A_1}, \underline{\Sigma}_{A_2}} \circ \langle \eta_{\underline{\Sigma}_{A_1}}, f_2 \rangle) \Big) \odot v_2', \tag{6.40}$$

in words, we extend v_2' by f_2. Lemmas 33 and 32 respectively imply

$$\mathscr{V}\pi_{\underline{\Sigma}_{A_1} \times \underline{\Sigma}_{A_2}} \circ v = v_2, \qquad \mathscr{V}\pi_{\underline{\Sigma}_{A_1} \times \underline{\Sigma}_{A_3} \times ... \times \underline{\Sigma}_{A_n}} \circ v = v_2'. \tag{6.41}$$

These equations state that the positive over pure tensor state corresponding to v has marginal states ρ_2 and ρ_2' overlapping at $\mathcal{H}_2$, which contradicts to the assumption that v_2 and v_2' corresponds to a non-extendible pair. We have proven that v_2 is a product valuation.

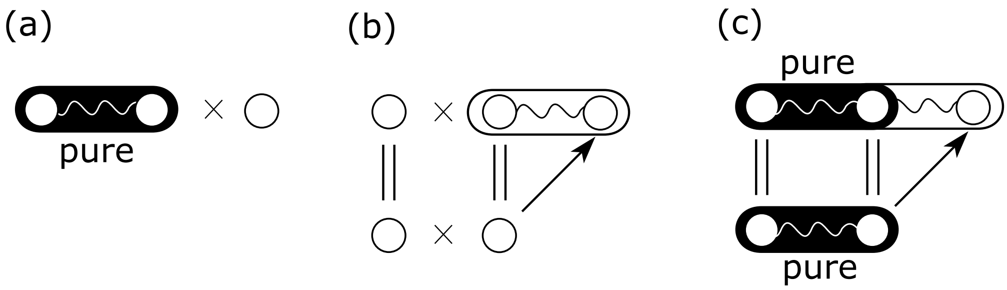

Figure 6.5: Three steps to show the triviality of our Markov chains. (a) If a bipartite marginal of a tripartite state is correlated and pure, the third party must be disconnected to the other two. (b) A Kleisli morphism which creates correlation. (c) The same Kleisli morphism extends a bipartite correlated pure state to a state contradicting to (a).

If v_{i-1} is a product valuation, it is decomposed to

$$v_{i-1} = i_{\underline{\Sigma}_{A_1}\times\ldots\times\underline{\Sigma}_{A_{i-2}},\underline{\Sigma}_{A_{i-1}}} \circ \langle w, w'\rangle, \tag{6.42}$$

where $w : 1 \to_{\mathcal{K}\ell} \underline{\Sigma}_{A_1} \times \ldots \times \underline{\Sigma}_{A_{i-2}}$, and $w' : 1 \to_{\mathcal{K}\ell} \underline{\Sigma}_{A_{i-1}}$ are valuations on the marginal systems and w is itself a product valuation. Lemma 31 suggests (cf. Eq. (6.6))

$$\begin{aligned} v_i &= \mathrm{ext}_i \odot v_{i-1} & (6.43)\\ &= i_{\underline{\Sigma}_{A_1}\times\ldots\times\underline{\Sigma}_{A_{i-2}},\underline{\Sigma}_{A_{i-1}}\times\underline{\Sigma}_{A_i}} \circ \langle w, (i_{\underline{\Sigma}_{A_{i-1}},\underline{\Sigma}_{A_i}} \circ \langle f_i, \eta_{\underline{\Sigma}_{A_{i-1}}}\rangle) \odot w'\rangle. & (6.44)\end{aligned}$$

Valuation v_i is now written as a product of w and

$$w'' := (i_{\underline{\Sigma}_{A_{i-1}},\underline{\Sigma}_{A_i}} \circ \langle f_i, \eta_{\underline{\Sigma}_{A_{i-1}}}\rangle) \odot w'. \tag{6.45}$$

It suffices to check that w'' is a product state since w is itself a product state. This can be shown in the same way of showing that v_2 is a product state. □

The core of this proof can be abstractly summarised as follows (see Fig. 6.5 alongside). Extremal bipartite non-product states cannot be extended to tripartite positive over pure tensor states so that it is not product between the original two and the third party (Fig. 6.5 (a)). If there should exist a map ext which extends product states to non-product positive over pure tensor states (Fig. 6.5 (b)), however, it would extend extremal bipartite non-product state to create the forbidden tripartite state (Fig. 6.5 (c)). The proof shows a fundamental incompatibility between our Markov chains and monogamy of states. Once a bijective correspondence between states defined by any commutative monad with $T1 \cong 1$ and quantum states (or positive over pure tensor states) on composite Hilbert spaces is established, the monogamy of quantum states (or positive over pure tensor states) immediately indicates the triviality of Markov chains.

The fundamental incompatibility between our Markov chains and the monogamy property stems from the cartesianness of the underlying category. Cartesianness of the underlying category enables us to construct morphisms

$$i \circ \langle f, g\rangle \tag{6.46}$$

by combining *arbitrary* Kleisli morphisms f and g. That means, every pair of Kleisli morphisms is compatible in the sense these two can be combined together to form a 1-to-2 map whose marginals coincides with the original pair. This is in contrast to the TPCP maps where a pair of two maps with the same domain is not necessarily compatible [105].

Remark 43. Theorem 42 also implies the non-existence of Kleisli morphisms $f : \underline{\Sigma}_{A_{i-1}} \to_{\mathcal{K}\ell} \underline{\Sigma}_{A_i}$ that create non-product states between $\underline{\Sigma}_{A_{i-1}}$ and $\underline{\Sigma}_{A_i}$. Typical morphisms that create only product states are

$$f_v : \underline{\Sigma}_{A_{i-1}} \xrightarrow{!_{\underline{\Sigma}_{A_{i-1}}}} 1 \xrightarrow{v} \mathscr{V}\underline{\Sigma}_{A_i}, \tag{6.47}$$

with the unique morphism $!_{\underline{\Sigma}_{A_{i-1}}}$ to the terminal object and any valuation $v : 1 \to_{\mathcal{K}\ell} \underline{\Sigma}_{A_i}$ on $\underline{\Sigma}_{A_i}$[6]. In words, f_v outputs a fixed state v no matter what the input is. If f_v is used for extension, it just adds state v as the last member of the Markov chain. Although we do not have a proof, we conjecture that the only Kleisli morphisms from $\underline{\Sigma}_{A_{i-1}}$ to $\underline{\Sigma}_{A_i}$ are those given by Eq. (6.47).

Remark 44. There is another generalisation of classical Markov chains to quantum theory, which exhibits classical correlations unlike our Markov chains for topos quantum theory. A tripartite quantum state $\rho_{XYZ} \in \mathcal{S}(\mathcal{H}_X \otimes \mathcal{H}_Y \otimes \mathcal{H}_Z)$ is a *short quantum Markov chain* [56] if there is a TPCP map $\mathcal{E}^{\rho_{XYZ}}_{Y\to YZ} : \mathcal{B}(\mathcal{H}_Y) \to \mathcal{B}(\mathcal{H}_Y \otimes \mathcal{H}_Z)$ such that

$$\rho_{XYZ} = \mathrm{id}_{\mathcal{H}_X} \otimes \mathcal{E}^{\rho_{XYZ}}_{Y\to YZ} \left(\mathrm{Tr}_{\mathcal{H}_Z}[\rho_{XYZ}]\right).$$

There are short quantum Markov chains which are not product in any partitioning. The trick to avoid the triviality forced by the monogamy is the dependency of $\mathcal{E}^{\rho_{XYZ}}_{Y\to YZ}$ on state ρ_{XYZ}. The map $\mathrm{id}_{\mathcal{H}_X} \otimes \mathcal{E}^{\rho_{XYZ}}_{Y\to YZ}$ extending chains preserves the marginal state $\mathrm{Tr}_{\mathcal{H}_Z}[\rho_{XYZ}]$ of ρ_{XYZ}, but it may change other input states from $\mathcal{S}(\mathcal{H}_X \otimes \mathcal{H}_Y)$. If $\mathcal{E}^{\rho_{XYZ}}_{Y\to YZ}$ must satisfy $\mathrm{Tr}_{\mathcal{H}_Z}[\mathrm{id}_{\mathcal{H}_X} \otimes \mathcal{E}^{\rho_{XYZ}}_{Y\to YZ}(\rho_{XY})] = \rho_{XY}$ for any state ρ_{XY} in $\mathcal{S}(\mathcal{H}_X \otimes \mathcal{H}_Y)$, $\mathcal{E}^{\rho_{XYZ}}_{Y\to YZ}$ separates to $\mathcal{E}_Y \otimes \Gamma_{\rho_Z}$ with a TPCP map $\mathcal{E}_Y : \mathcal{B}(\mathcal{H}_Y) \to \mathcal{B}(\mathcal{H}_Y)$ and $\Gamma_{\rho_Z} : \mathcal{B}(\mathbb{C}) \to \mathcal{B}(\mathcal{H}_Z)$ to prepare state ρ_Z, and the resulting short quantum Markov chain is product, much like our Markov chains for topos quantum theory.

[6] These morphism always exist since v correspond to valuations, and $!_{\underline{\Sigma}_{A_{i-1}}}$ always exists.

Chapter 7

Conclusion and outlook

We have considered two kinds of theories as an intermediate theory between quantum and classical probability theory, and studied the gap between positive and CP maps in the intermediate theories. On the first approach, the linearity constraint, which does not exist on classical maps, are removed from quantum maps by considering non-linear resources such as cloned states and replicated channels. We have analysed realisability of positive non-CP maps and supermaps with these extra resources. On the second approach, we have investigated maps in topos quantum theory by considering states on composite systems and Markov chains.

About the positive non-CP maps, we have obtained no-go theorems for probabilistic realisation of positive non-CP maps from finite clones of the input states. It is impossible to produce the output state of several positive non-CP maps including the state transposition, from given finite clones of the unknown input state uncorrelated to other systems. In this sense, the gap between positive and CP maps does not completely close with only a limited power of non-linearity added to quantum theory.

There still remains much unsolved on the power of non-linearity for realising positive non-CP maps. Positive non-CP maps not satisfying the condition of Lem. 9 may be possibly probabilistically realised from finite clones. Although the author is pessimistic about the possibility, these classes of positive non-CP maps are worth studying for the complete analysis on the gap between positive and CP maps. Another open question is the probabilistic realisability of positive non-CP maps from clones of *pure* input states. State transposition is shown unrealisable even if the input state is chosen from pure states. In contrast, Lem. 9 denies a probabilistic realisability of certain positive non-CP maps, where the input state is chosen from arbitrary quantum states uncorrelated to other systems. It is open if those maps remain unrealisable if the input states are restricted to pure states.

When we consider probabilistic realisability of positive non-CP supermaps, the difference between pure and noisy input TPCP maps is not negligible. We have considered probabilistic realisability of particular positive non-CP supermap, namely the channel transposition, with and without replication of the input TPCP maps uncorrelated to other systems in the Choi operator representations. Since the channel transposition on general TPCP maps includes state transposition, it is not realisable from finite replicas of general input TPCP maps. However, if the input TPCP map is restricted to unitary channels, which can be regarded as pure

TPCP maps, the channel transposition reduces to unitary conjugation, and it is realisable from finite replicas of the unitary channel. Specifically, we have shown that the unitary conjugation is not realisable without replicas if the dimension of the Hilbert space is more than 2, and presented the pair of the encoder and the decoder that, together with $d(d-1)$ replicas of the unknown unitary channel, implements the single conjugated unitary channel.

Thus we see that some of the gap between positive and CP supermaps is filled with only finite power of non-linearity. In contrast to the state transposition, finite non-linearity is helpful for channel transposition on noiseless TPCP maps. In this way, we have obtained an evidence that positive non-CP supermaps may behave differently to the corresponding maps.

Our scheme to realise unitary conjugation has a clear physical interpretation. When fermions undergo a mode transformation represented by a unitary operator on the single particle space, corresponding holes are transformed according to the conjugated unitary operator. Our unitary conjugation scheme is essentially equivalent to this phenomena when the fermionic systems and antisymmetric subspaces of Hilbert spaces are identified.

Besides the investigation on the gap between positive and CP maps, we have obtained a method to construct observables for conjugation induced quantities by applying an observation gained from the analysis on the channel transposition. We have defined a class of conjugation induced quantities associated to linear maps, and showed observables whose expectation values coincide with these quantities. The class of conjugation induced quantity is large enough to include many known quantities, such as concurrence, 3-tangle, and I-concurrence. For a restricted class defined by filters [77], our observable coincides with those presented in Ref. [81]. A family of concurrence monotones including the G-concurrence presented in Ref. [69] has found the expression as conjugation induced quantities and, at the same time, the corresponding observables presented in Ref. [71] are rediscovered. Our construction of observables shows a fundamental equivalence between observable local unitary invariants [80, 71] and conjugation induced local unitary invariants, and clarifies why conjugation often appears in multipartite correlation measures.

With our observables, conjugation induced quantities are directly measurable from clones of the state, without requiring the recourse of state tomography. It is still open if our observables can measure measure these quantities more efficiently compared to state tomography. The solution of this problem would depend on the quantities of interest, and also on the definition of "efficiency," which would reflect requirements from specific experimental setups. While our observables are constructed for a broad class of conjugation induced quantities and do not depend on experimental setups, more details should be studied on individual settings.

We have not studied realisability of different positive non-CP maps other than channel transposition. Other examples of positive non-CP supermaps would be provided by recent works on tensor stability of positive maps [16, 17]. It is an interesting open problem if there is a positive non-CP supermap realisable from finite replicas of unitary channels, other than channel transposition. At this moment, it is not clear that the realisability from finitely replicated unitary channels is a universal property shared by all positive non-CP supermaps, or channel transposition is special among them.

To summarise the first approach, we have shown that finite number of clones and replicas of the inputs are not enough to realize several positive non-CP maps and the supermap. From this result we may conclude that the gap between positive and CP maps reflects the difference between finite and infinite clones provided as inputs, rather than the difference between null and finite ones. On the other hand, a non-trivial restriction on the space of inputs is shown to provide an opportunity for a positive non-CP *supermap* to be realized from finite replicas of the inputs, while the similar restriction on the input space of the analogous positive non-CP *map* does not help. Thus from the analysis on the gap between positivity and complete positivity in the intermediate between quantum theory and classical probability theory, we deduce an implication on the quantum theory itself that positive non-CP maps and supermaps may behave differently under certain condition.

The second approach taken in this thesis on the gap of maps is complementary to the first one, in that the second approach starts from classical probability theory while the first one from quantum theory. We tried to see which of the positive and CP maps appear when topos quantum theory generalises classical theory to describe quantum systems. We have not obtained the result that directly answers this question, but made several observations that relate notions of positivity in quantum theory and that in topos quantum theory.

We defined composite systems in topos quantum theory, by generalising products of random variables representing the composite systems in classical probability theory. From toposes and their internal commutative C*-algebras describing marginal quantum systems, a unifying topos is first constructed, and the coproduct of C*-algebras is taken in the unifying topos, as done for bipartite systems in Ref. [47]. Taking coproducts of C*-algebras is equivalent to taking product of corresponding locales. The joint valuations on product locales and, equivalently, the integrals over coproduct algebras have bijective correspondence between positive over pure tensor states instead of quantum states.

The gap between joint valuations and quantum states arises since the joint valuations are not required to be positive on entangled positive operators, while quantum states are. This is because our coproducts of commutative C*-algebras lack the commutative C*-subalgebra for entangled observables. It is open if there exists another definition of composite systems leading a bijective correspondence between joint valuations and quantum states. Commutative C*-algebras for such a composition would include sufficient commutative subalgebras for entangled observables.

Our analysis reveals that there is no unique way to generalise composite systems of classical probability theory to topos quantum theory. This arbitrariness arises in the first place from the use of different toposes for describing marginal quantum systems. All random variables in classical probability theory are objects in unique topos **Sets**, while the marginal locales of topos quantum theory may exist in different toposes.

The Kleisli morphisms of the valuation monad are regarded to be maps in topos quantum theory, and we have investigated its behaviour on composite systems. The commutativity of valuation monad alone implies that the Kleisli morphisms are CP in the sense that arbitrary two Kleisli morphisms acting in parallel generate valid Kleisli morphisms. This does not imply, however, that positive non-CP quantum maps are excluded from the Kleisli morphisms of the valuation monad. Since joint valuations corresponding to positive over pure tensor states are regarded as states in our definition of composite systems, actions of positive non-CP maps on a part of entangled states produces valid states in topos quantum theory. The definition of complete positivity for topos quantum theory highly depends on how to define composite systems.

We generalised classical Markov chains directly to topos quantum theory, by replacing distribution monad (used in classical probability theory) to valuation monad (used in topos quantum theory). The Markov chains are recursively defined by extending short Markov chains by Kleisli morphisms of valuation monad. We have shown a fundamental incompatibility between our Markov chains and the monogamy property of positive over pure tensor states, and demonstrated that our Markov chains correspond only to product valuations on composite systems. Markov chains in topos quantum theory is more trivial than classical ones which can contain classical correlation. This consequence reveals that there only exist maps between different marginal systems that do not create correlation in topocs quantum theory. Kleisli morphisms between different marginal systems seems to be too trivial to ask complete positivity.

This triviality of Markov chains has two origins: the use of (cartesian) product to describe composite systems, and $1 \cong \mathscr{V}1$ for the valuation monad. It is sometimes considered that the product may not be suitable for describing composition for quantum systems [106]. The triviality of our Markov chains reinforces this observation, by showing an incompatibility between product and the monogamy existing in quantum states and positive over pure tensor states. While we cannot define our Markov chains without the product, $1 \cong \mathscr{V}1$ is not a crucial property. It might be interesting to consider our Markov chains for different monad T and cartesian category other than the valuation monad on category of locales, such that $1 \ncong T1$.

To avoid the triviality of the Kleisli morphisms of the valuation monad between different marginal systems, the composite systems in topos quantum theory have to be taken by non-cartesian tensor product of locales. Our analysis on the maps thus reveals that the definition of composite systems by cartesian products cannot be directly extended from classical probability theory. This non-extendibility applies not only to topos quantum theory, but to any theory using commutative monads with $T1 \cong 1$ to describe a quantum-like system with the monogamy property as we have mentioned just after Thm. 42. While we do not find any suitable definition of the tensor product between locales, it is worth trying for further development of topos quantum theory.

To summarise the second approach, we have defined composite systems of topos quantum theory by generalising the cartesian product of random variables in classical probability theory, and showed that positive non-CP maps is regarded as valid transformations on valuations there, even if they act in parallel with identity maps. It is possible to exclude the positive non-CP maps from valid state transformations if one can employ a different definition of composite systems where the joint valuations have bijective correspondence between multipartite quantum states. While we currently do not find any definition of composite system exhibiting this bijection, the composite should be taken by a non-cartesian tensor product of locales, since maps connecting each sides of a cartesian product may have a trivial structure. Our understanding on the difference between quantum theory and classical probability theory is sharpened by revealing an incompatibility between the composition in classical probability theory and non-trivial state transformations in topos quantum theory.

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Appendix A

Hilbert space of operators

The set of operators $\mathcal{B}(\mathcal{H})$ on finite dimensional Hilbert spaces is itself a Hilbert space. Using the structure of this Hilbert space, we review that it is possible calculate the description of unknown quantum state from outcome probabilities of several measurements (mentioned in Sec. 1.1.2), introduce the operator Schmidt decomposition (used in the proof of Thm. 11), and introduce Hermitian adjoints in operator Hilbert spaces (used in Sec. 2.1.1).

The space $\mathcal{B}(\mathcal{H})$ of linear operators on $\mathcal{H}$ is a Hilbert space with the Hilbert-Schmidt inner product

$$(A, B)_{\mathrm{HS}} := \mathrm{Tr}[A^\dagger B] \qquad (A, B \in \mathcal{B}(\mathcal{H})). \tag{A.1}$$

The dimension of this space is d^2 where $\dim \mathcal{H} = d$. There always exists a set of Hermitian operators $\{O_i\}_{i=1,\ldots,(\dim \mathcal{H})^2}$ that forms a complete orthonormal basis of this inner product.

These Hermitian operators provides a method to obtain the description of an unknown quantum state. Any state $\rho \in \mathcal{S}(\mathcal{H})$ is decomposed into

$$\rho = \sum_i^{(\dim \mathcal{H})^2} O_i (O_i, \rho)_{\mathrm{HS}} = \sum_i^{(\dim \mathcal{H})^2} O_i \mathrm{Tr}[O_i \rho]. \tag{A.2}$$

in terms of the Hermitian operators. From a collection of the expectation values $\{\mathrm{Tr}[O_i\rho]\}$ of Hermitian operators, the description of state ρ is calculated by Eq. (A.2). Implementation of the measurements to evaluate the expectation values of O_i on infinitely many clones of the unknown state ρ reveals the description of the unknown states.

If there are two operator spaces $\mathcal{B}(\mathcal{H})$ and $\mathcal{B}(\mathcal{K})$, their tensor product $\mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathcal{K})$ can be also taken as Hilbert spaces. Elements of $\mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathcal{K})$ are equivalent to those in $\mathcal{B}(\mathcal{H} \otimes \mathcal{K})$ by definition. This enables the Schmidt decomposition (see Sec. 2.3.2 for the definition) of operators in $\mathcal{B}(\mathcal{H} \otimes \mathcal{K})$ in the bi-partition $\mathcal{B}(\mathcal{H})$-$\mathcal{B}(\mathcal{K})$, which is called as the operator Schmidt decomposition. Explicitly, for any operator $a \in \mathcal{B}(\mathcal{H} \otimes \mathcal{K})$, there exist sets of operators $\{\gamma_i^{\mathcal{H}}\}_{i=1,\ldots,\dim \mathcal{H}}$ and $\{\gamma_i^{\mathcal{K}}\}_{i=1,\ldots,\dim \mathcal{K}}$ that forms an orthonormal basis in $\mathcal{B}(\mathcal{H})$ and $\mathcal{B}(\mathcal{K})$, respectively, where the orthonormality is defined by the Hilbert-Schmidt inner product of each operator space, such that

$$a = \sum_i r_i \, \gamma_i^{\mathcal{H}} \otimes \gamma_i^{\mathcal{K}}. \tag{A.3}$$

with a family of non-negative numbers $\{r_i\}$.

The Hermitian adjoints in operator Hilbert spaces provide a duality between maps in $\mathcal{B}(\mathcal{B}(\mathcal{H}), \mathcal{B}(\mathcal{K}))$ and $\mathcal{B}(\mathcal{B}(\mathcal{K}), \mathcal{B}(\mathcal{H}))$. Let $\mathcal{F} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ be a linear map. In other words, $\mathcal{F}$ is an operator from Hilbert space $\mathcal{B}(\mathcal{H})$ to $\mathcal{B}(\mathcal{K})$. The Hermitian adjoint $\mathcal{F}^\dagger : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ of $\mathcal{F}$ is defined by

$$(\mathcal{F}^\dagger(A), B))_{\mathrm{HS}} = (A, \mathcal{F}(B))_{\mathrm{HS}} \qquad (\forall A \in \mathcal{B}(\mathcal{K}),\ \forall B \in \mathcal{B}(\mathcal{H})). \tag{A.4}$$

If $\mathcal{F}$ is positive, then $\mathcal{F}^\dagger$ is also positive since

$$\mathrm{Tr}[\mathcal{F}^\dagger(\rho)\sigma] = (\mathcal{F}^\dagger(\rho), \sigma)_{\mathrm{HS}} = (\rho, \mathcal{F}(\sigma))_{\mathrm{HS}} = \mathrm{Tr}[\rho\mathcal{F}(\sigma)] \geq 0 \tag{A.5}$$

holds for any pair of positive semi-definite operators $\rho \in \mathrm{Pos}(\mathcal{K})$ and $\sigma \in \mathrm{Pos}(\mathcal{H})$.

Appendix B

Operator $A_{n\to m}$ and its variants

In this appendix we show several properties of operators concerning to antisymmetric subspaces, which find their use in Chap. 4[1]. We restate the definition of operator $A_{i_1,\ldots,i_{n+m}} : \mathcal{H}^{\otimes n} \to \mathcal{H}^{\otimes m}$ $(1 \leq i_1 < \ldots < i_{m+n} \leq d)$ presented by Eq. (4.67) again,

$$A_{i_1,\ldots,i_{n+m}} := \frac{1}{\sqrt{(n+m)!}} \sum_{\tau \in \mathrm{S}_{n+m}} \mathrm{sgn}(\tau) |\tau_{i_1}, \ldots, \tau_{i_m}\rangle\langle\tau_{i_{m+1}}, \ldots, \tau_{i_{m+n}}|, \tag{B.1}$$

where S_{n+m} represents the symmetry group of order $m+n$. If $m+n = d := \dim \mathcal{H}$, $A_{i_1,\ldots,i_{n+m}}$ is given by $A_{1,2,\ldots,d}$ and it coincides with $\frac{m!n!}{(m+n)!} A_{n\to m}$ defined by Eq. (4.26).

B.1 General properties

In this section, we first show that that $A_{n\to m}$ is a unitary operator connecting antisymmetric subspaces $\mathcal{H}^{\wedge n}$ to $\mathcal{H}^{\wedge m}$. This property is used in the construction of supermap implementing conjugate unitaries in Sec. 4.2.2. Second, we show that the Choi operator for CP map $S' : \mathcal{B}(\mathcal{H}^{\otimes n}) \to B(\mathcal{H}^{\otimes m})$ with Kraus decomposition

$$S' = \sum_{1 \leq i_1 < \ldots < i_{m+n} \leq d} \mathcal{U}[A_{i_1,\ldots,i_{m+n}}], \tag{B.2}$$

is a projector onto antisymmetric subspace. This is used in the proof of Lem. 14, and also for obtaining observables for a conjugation induced quantity in Sec. 2.3.4.

Operator $A_{n\to m} : \mathcal{H}^{\otimes n} \to \mathcal{H}^{\otimes m}$ is defined by

$$\begin{aligned} A_{n\to m} &:= \frac{1}{\sqrt{m!n!}} \sum_{\tau \in \mathrm{S}_{m+n}} \mathrm{sgn}(\tau) |\tau_1, \ldots, \tau_m\rangle\langle\tau_{m+1}, \ldots, \tau_{m+n}| && \text{(B.3)} \\ &= \frac{(-1)^{mn}}{\sqrt{m!n!}} \sum_{\tau \in \mathrm{S}_{m+n}} \mathrm{sgn}(\tau) |\tau_{n+1}, \ldots, \tau_{n+m}\rangle\langle\tau_1, \ldots, \tau_n|. && \text{(B.4)} \end{aligned}$$

Each element $\tau \in \mathrm{S}_{m+n}$ is uniquely decomposed to $\tau = (\tau^n \otimes \tau^m) \circ \nu$, where $\nu \in \mathrm{S}_{m+n}$ is restricted by

$$\nu_1 < \ldots < \nu_n, \; \nu_{n+1} < \ldots < \nu_{n+m}, \tag{B.5}$$

[1]The content of Appx. B is presented in Ref. [84]

and τ^n (τ^m) represents a permutation inside $\nu_1, ..., \nu_n$ ($\nu_{n+1}, ..., \nu_{n+m}$). Denoting the set of permutations satisfying Eq. (B.5) by $\mathrm{T}_{n,m}$, $A_{n\to m}$ is rewritten as

$$\begin{aligned} & A_{n\to m} \\ = \; & \frac{(-1)^{mn}}{\sqrt{n!m!}} \sum_{\nu\in T_{n,m}} \mathrm{sgn}(\nu) \sum_{\tau^n\in \mathrm{S}_n,\ \tau^m\in\mathrm{S}_m} \mathrm{sgn}(\tau^m)\mathrm{sgn}(\tau^n)|\tau^m_{\nu_{n+1}}, ..., \tau^m_{\nu_{n+m}}\rangle\langle\tau^n_{\nu_1}, ..., \tau^n_{\nu_n}| \\ = \; & (-1)^{mn} \sum_{\nu\in T_{n,m}} \mathrm{sgn}(\nu)|\wedge_{\nu_{n+1},...,\nu_{n+m}}\rangle\langle\wedge_{\nu_1,...,\nu_n}| \\ = \; & (-1)^{mn} \sum_{\nu\in T_{n,m}} (-1)^{n(n+1)/2+\sum_{k=1}^n \nu_k}|\wedge_{\nu_{n+1},...,\nu_{n+m}}\rangle\langle\wedge_{\nu_1,...,\nu_n}|, \end{aligned} \tag{B.6}$$

where we have used $\mathrm{sgn}(\nu) = (-1)^{\sum_{k=1}^n(\nu_k-k)} = (-1)^{n(n+1)/2+\sum_{k=1}^n \nu_k}$ to obtain the third equality. The expression of $A_{n\to m}$ presented in Eq. (B.6) implies that the $A_{n\to m}$ is a unitary operator between antisymmetric subspaces $\mathcal{H}^{\wedge n}$ and $\mathcal{H}^{\wedge m}$. Note that $\dim \mathcal{H}^{\wedge m} = \binom{d}{m} = \binom{d}{n} = \dim \mathcal{H}^{\wedge n}$.

The Choi operators of CP map S' presented by Eq. (B.2) is defined to be

$$\widetilde{S'} = \mathrm{id}_{\mathcal{H}^{\bullet n}} \otimes S'(\Phi^{\bullet n}_{\mathcal{H}\otimes\mathcal{H}}), \tag{B.7}$$

where we denote the tensor products for the bi-partition of the Choi operator by usual $\otimes$, and those for copied spaces by $\bullet$. $\Phi_{\mathcal{H}\otimes\mathcal{H}}$ denotes the density operator for the unnormalised maximally entangled state $\sum_{i=1}^d |i,i\rangle$. Note that the choice of state $\sum_{i=1}^d |i,i\rangle$ for defining the Choi operator is determined by the choice of the basis for complex conjugation. A straightforward calculation shows

$$\begin{aligned} & \widetilde{S'} \\ = \; & \mathrm{id}_{\mathcal{H}^{\bullet n}} \otimes \sum_{1\le i_1<...<i_{m+n}\le d} \mathcal{U}[A_{i_1,...,i_{m+n}}](\Phi^{\bullet n}_{\mathcal{H}\otimes\mathcal{H}}) \\ = \; & \sum_{1\le i_1<...<i_{m+n}\le d} \mathcal{U}[\mathbb{I}_{\mathcal{H}^{\otimes n}} \otimes A_{i_1,...,i_{m+n}}](\Phi^{\bullet n}_{\mathcal{H}\otimes\mathcal{H}}) \\ = \; & \sum_{1\le i_1<...<i_{m+n}\le d} \\ & \left(\sum_{\tau\in\mathrm{S}_{n+m}} \sum_{j_1,...,j_m=1}^{d} \frac{\mathrm{sgn}(\tau)\langle\tau_{i_{n+1}}|j_1\rangle...\langle\tau_{n+m}|j_m\rangle}{\sqrt{(n+m)!}}|\tau_{i_1}, ..., \tau_{i_n}\rangle \otimes |j_1, ..., j_m\rangle\right)(h.c.) \\ = \; & \sum_{1\le i_1<...<i_{m+n}\le d} \left(\sum_{\tau\in\mathrm{S}_{n+m}} \frac{\mathrm{sgn}(\tau)}{\sqrt{(n+m)!}}|\tau_{i_1}, ..., \tau_{i_n}\rangle \otimes |\tau_{n+1}, ..., \tau_{n+m}\rangle\right)(h.c.) \\ = \; & \sum_{1\le i_1<...<i_{m+n}\le d} |\wedge_{i_1,...,i_{n+m}}\rangle\langle\wedge_{i_1,...,i_{n+m}}|, \\ = \; & \Pi_{\mathcal{H}^{\wedge n+m}} \end{aligned}$$

where $(h.c.)$ represents the hermitian conjugate of the elements just before them. Thus we have shown that the Choi operator for S' defined by Eq. (B.2) coincides with the projector onto antisymmetric subspace.

B.2 Evaluation of local unitary invariants

In this section, we prove Eq. (4.70) by explicitly calculating

$$\mathrm{C}_{S'}(\rho) := \mathrm{Tr}\left[\rho^{\bullet m} S'(\rho^{*\bullet m})\right] \tag{B.8}$$

$$= \mathrm{Tr}[\rho^{\bullet m+n}\Pi_{\mathcal{H}^{\wedge m+n}}]. \tag{B.9}$$

Without loss of generality we can assume that the input state $\rho \in \mathcal{S}(\mathcal{H})$ is diagonalised $\rho = \sum_{i=1}^{d} p_i |i\rangle\langle i|$ in the computational basis, since $\mathrm{C}_{S'}(\rho)$ is unitary invariant. By decomposing $\Pi_{\mathcal{H}^{\wedge m+n}}$, we obtain

$$\mathrm{C}_{S'}(\rho) = \sum_{1\le i_1<\ldots<i_{n+m}\le d} \mathrm{Tr}\left[|\wedge_{i_1,\ldots,i_{n+m}}\rangle\langle\wedge_{i_1,\ldots,i_{n+m}}|\rho^{\bullet n+m}\right],$$

and each component of the summation is calculated as

$$\begin{aligned}
&\mathrm{Tr}[|\wedge_{i_1,\ldots,i_{n+m}}\rangle\langle\wedge_{i_1,\ldots,i_{n+m}}|\rho^{\bullet n+m}] \\
=\ & \frac{1}{(n+m)!}\sum_{j_1,\ldots,j_{n+m}=1}^{d} p_{j_1}\ldots p_{j_{n+m}}\langle j_1,\ldots,j_{n+m}| \\
&\left(\sum_{\sigma,\tau\in \mathrm{S}_{n+m}} \mathrm{sgn}(\sigma)\mathrm{sgn}(\tau)|\sigma(i_1),\ldots,\sigma(i_{n+m})\rangle\langle\tau(i_1),\ldots,\tau(i_{n+m})|\right)|j_1,\ldots,j_{n+m}\rangle \\
=\ & \frac{1}{(n+m)!}\sum_{\sigma\in \mathrm{S}_{n+m}} (\mathrm{sgn}(\sigma))^2 p_{\sigma(i_1)}\ldots p_{\sigma(i_{n+m})} = p_{i_1}\ldots p_{i_{n+m}}.
\end{aligned}$$

Summing up all the components, we obtain

$$\mathrm{C}_{S'}(\rho) = \sum_{1\le i_1<\ldots<i_{n+m}\le d} p_{i_1}\ldots p_{i_{n+m}}. \tag{B.10}$$

These quantities for $n+m = 1,\ldots,d$ are Schur concave [107], and thus they measure how mixed the state is. In particular, the second of the family C_2^1 is a monotonic function of purity $\sqrt{1-\mathrm{Tr}[\rho^2]}$.

For pure states quantities $\mathrm{C}_{S'\otimes S'}$ become good measures of entanglement. For mixed states, however, they are not necessary measuring entanglement since for example, they may have positive values on product mixed states.

B.3 Particle-hole exchange operator

In this section, we show that the operator $A_{n\to m}$ is equivalent (up to phase) to the particle-hole exchange operator E_n^d in fermion systems. This completes our interpretation of unitary conjugation in fermion systems presented in Sec. 4.2.3.

Let $\mathcal{H}$ be a d-dimensional Hilbert space with a basis $\{|i\rangle\}_{i=1,\ldots,d}$. Let us consider identical fermions whose internal degree of freedom described by $\mathcal{H}$. We denote the operator annihilating a fermion in state $|\psi\rangle$ by $a_{|\psi\rangle}$. The vacuum and completely occupied states are denoted by $|\mathrm{vac}\rangle$ and

$$|\mathrm{occ}\rangle := a_{|1\rangle}^{\dagger}\ldots a_{|d\rangle}^{\dagger}|\mathrm{vac}\rangle, \tag{B.11}$$

respectively. The antisymmetric subspace $\mathcal{H}^{\wedge n}$ of $\mathcal{H}^{\otimes n}$ is identified with n-fermion Fock space by the equivalence relation

$$|\wedge_{i_1,\ldots,i_n}\rangle := \frac{1}{\sqrt{n}} \sum_{\tau \in \mathrm{S}_n} \mathrm{sgn}(\tau) |\tau_{i_1}, \ldots, \tau_{i_n}\rangle \sim |\Psi^{\mathrm{particle}}_{i_1,\ldots,i_n}\rangle := a^\dagger_{|i_1\rangle} \ldots a^\dagger_{|i_n\rangle} |\mathrm{vac}\rangle, \quad \text{(B.12)}$$

where S_n represents the symmetric group of order n.

We show that particle hole exchange operator is equivalent to operator $A_{n\to m}$ under the identification of fermion systems and antisymmetric subspaces. An n-hole state is related to a $d-n$-particle state by

$$\begin{aligned} |\Psi^{\mathrm{hole}}_{i_1,\ldots,i_n}\rangle &:= a_{|i_1\rangle} \ldots a_{|i_n\rangle} |\mathrm{occ}\rangle, && \text{(B.13)} \\ &= (-1)^{i_n - 1} a_{|i_1\rangle} \ldots a_{|i_{n-1}\rangle} a^\dagger_{|1\rangle} \ldots \hat{a}^\dagger_{|i_n\rangle} \ldots a^\dagger_{|d\rangle} |\mathrm{vac}\rangle && \text{(B.14)} \\ &= \ldots && \text{(B.15)} \\ &= (-1)^{\sum_{k=1}^n (i_k - 1)} a^\dagger_{|1\rangle} \ldots \hat{a}^\dagger_{|i_1\rangle} \ldots \hat{a}^\dagger_{|i_n\rangle} \ldots a^\dagger_{|d\rangle} |\mathrm{vac}\rangle && \text{(B.16)} \\ &= (-1)^{n - \sum_{k=1}^n i_k} |\Psi^{\mathrm{particle}}_{i_1,\ldots,\hat{i_1},\ldots,\hat{i_n},\ldots,i_d}\rangle, && \text{(B.17)} \end{aligned}$$

where elements with hat $\hat{\cdot}$ are absent from the sequences. The particle-hole exchange operator E^d_n is defined by

$$E^d_n := \sum_{1 \le i_1 < \ldots < i_n \le d} |\Psi^{\mathrm{hole}}_{i_1,\ldots i_n}\rangle \langle \Psi^{\mathrm{particle}}_{i_1,\ldots,i_n}|, \quad \text{(B.18)}$$

and is equivalent to

$$(-1)^n \sum_{1 \le i_1 < \ldots < i_n \le d} (-1)^{\sum_{k=1}^n i_k} |\wedge_{1,\ldots,\hat{i_1},\ldots,\hat{i_n},\ldots,d}\rangle \langle \wedge_{i_1,\ldots,i_n}|. \quad \text{(B.19)}$$

On the other hand, operator $A_{n\to m} : \mathcal{H}^{\otimes n} \to \mathcal{H}^{\otimes m}$ is represented by Eq. (B.6). By comparing Eqs. (B.19) and (B.6), we obtain

$$E^d_n \sim (-1)^{n(n-1)/2 + mn} A_{n\to m}. \quad \text{(B.20)}$$

Appendix C

Category theory

C.1 Definitions

This section reviews basic definitions in category theory (see e.g. [108] for more detail). Full understanding of Chap. 6 also requires slightly advanced notions reviewed in Sec.C.2 and Sec. C.3. Full understanding of Chap. 5 requires the notions from topos theory reviewed in Sec. C.4.

objects and morphisms A category constitutes of a collection of *objects* and *morphisms* (or maps or arrows). Each morphism f in a category has its domain object and codomain object, denoted by $\mathrm{dom}(f)$ and $\mathrm{cod}(f)$ respectively. If there is a morphism with $\mathrm{dom}(f) = A$ and $\mathrm{cod}(f) = B$, we write

$$f : A \to B.$$

A collection of all morphisms from A to B on a category $\mathbf{C}$ is denoted by $\mathrm{Hom}_{\mathbf{C}}(A, B)$. If $f : A \to B$ and $g : B \to C$, a composition morphism $g \circ f : A \to C$ must be defined on the category. The associativity $h \circ (g \circ f) = (h \circ g) \circ f$ must hold.

isomorphisms A morphism $f : A \to B$ is called an isomorphism if there exists an inverse of f, denoted by $g : B \to A$, which satisfies both $f \circ g = \mathrm{id}_B$ and $g \circ f = \mathrm{id}_A$. If there is an isomorphism between objects A and B, then they are said to be isomorphic.

dual category A dual category $\mathbf{C}^{op}$ of $\mathbf{C}$ is a category which has the same collection of objects to $\mathbf{C}$, the same collection of morphisms to $\mathbf{C}$ but each morphism has the opposite direction.

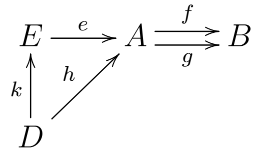
terminal and initial object A terminal object denoted by 1 is an object such that for all object A there is a unique morphism $!_A : A \to 1$. The terminal object is unique up to isomorphism.

The initial object is the terminal object in dual category. An initial object denoted by 0 is an object such that for all object A there is a unique morphism $0 \to A$.

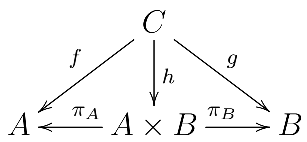
equaliser An equaliser of two morphisms $f, g : A \to B$ is a pair of an object E and morphism $e : E \to A$ that satisfies following two conditions:

1. $f \circ e = g \circ e$,

2. for any morphism $h : D \to A$ such that $f \circ h = g \circ h$, there exists a unique morphism k such that the following diagram commutes:

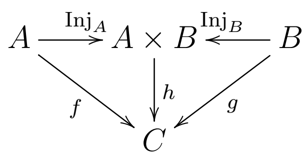


product and coproduct An object denoted by $A \times B$ satisfying following two conditions is called the product of objects A and B. (i) There are morphisms $\pi_A : A \times B \to A$ and $\pi_B : A \times B \to B$. (ii) For all $C,\ f : C \to A,\ g : C \to B$, there exists a unique morphism $h : C \to A \times B$ such that,

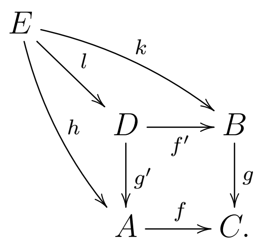


We denote the unique morphism h by $\langle f, g \rangle$.

Coproduct is product in the dual category. An object $A \coprod B$ satisfying following two conditions is called the coproduct of objects A and B. (i) There are morphisms $\mathrm{Inj}_A : A \to A \coprod B$ and $\mathrm{Inj}_B : B \to A \coprod B$. (ii) For all $C,\ f : A \to C,\ g : B \to C$, there exists a unique morphism $h : A \coprod B \to C$ such that,



pullback $A \overset{g'}{\leftarrow} D \overset{f'}{\rightarrow} B$ is a pullback of $A \overset{f}{\rightarrow} D \overset{g}{\leftarrow} B$ if $g \circ f' = f \circ g'$ and for all object E, $h : E \to A$, $k : E \to B$ satisfying $f \circ h = g \circ k$, there exists a unique morphism $l : E \to D$ such that the following commutative diagram holds.



sub-object classifier Let $\mathbf{C}$ be a category with a terminal object 1. An object Ω is called a sub-object classifier if there exists a morphism $T : 1 \to \Omega$ such that $\forall f : A \rightarrowtail B$, $^{\exists!}\chi_f : B \to \Omega$ that make next commutative diagram a pullback:

$$\begin{array}{ccc} A & \xrightarrow{!_A} & 1 \\ {\scriptstyle f}\big\downarrow & & \big\downarrow{\scriptstyle T} \\ B & \xrightarrow[\chi_f]{} & \Omega \end{array}$$

functor Let $\mathbf{C}$ and $\mathbf{D}$ be categories. A *covariant functor* $F : \mathbf{C} \to \mathbf{D}$ is a map that assigns $\mathbf{D}$-object F_C for every $\mathbf{C}$-object C and $\mathbf{D}$-morphism $F(f) : F(A) \to F(B)$ for every $\mathbf{C}$-morphism $f : A \to B$ in the following way:

1. if $\mathrm{cod}(f) = \mathrm{dom}(g)$ for two $\mathbf{C}$-morphisms f and g, $F(g \circ f) = F(g) \circ F(f)$,
2. $F(\mathrm{id}_C) = \mathrm{id}_{F_C}$ for any $\mathbf{C}$-object C.

A *contravariant functor* from $\mathbf{C}$ to $\mathbf{D}$ is a covariant functor from $\mathbf{C}^{op}$ to $\mathbf{D}$. Note that the contravariant functor changes the direction of morphisms. A contravariant functor from $\mathbf{C}$ to $\mathbf{Sets}$ is often called a *presheaf* on $\mathbf{C}$.

Natural transformations A natural transformation from a functor X to a functor Y, $N : X \to Y$, is a collection of maps $N_A : X_A \to Y_A$ such that the following diagram commutes:

$$\begin{array}{ccc} X_A & \xrightarrow{X(f)} & X_B \\ {\scriptstyle N_A}\big\downarrow & & \big\downarrow{\scriptstyle N_B} \\ Y_A & \xrightarrow{Y(f)} & Y_B. \end{array}$$

Note that no element of a natural transformation is defined on the elements of the form $X(f)$.

Functors and natural transformations forms a category. If $\mathbf{C}$ and $\mathbf{D}$ are categories, $[\mathbf{C}, \mathbf{D}]$ denotes the category which has functors from $\mathbf{C}$ to $\mathbf{D}$ as objects and natural transformations between them as morphisms.

C.2 Symmetric monoidal and cartesian categories

Symmetric monoidal and cartesian categories are categories with certain structures. We use these categories for considering Markov chains in Chap. 6. Here we review their definitions. While we do not use defining properties of symmetric monoidal categories explicitly in this thesis, we quote several theorems.

Definition 45. A monoidal category is a category $\mathbf{C}$ with

- a functor $\otimes : \mathbf{C} \times \mathbf{C} \to \mathbf{C}$ called "tensor product,"
- an object I called "unit,"

- a natural isomorphism $\alpha_{X,Y,Z} : (X \otimes Y) \otimes Z \xrightarrow{\sim} X \otimes (Y \otimes Z)$ called the "associator,"
- natural isomorphisms $l_X : I \otimes X \xrightarrow{\sim} X$ and $r_X : X \otimes I \xrightarrow{\sim} X$ respectively called "left unitor" and "right unitor,"

such that following diagrams commute for all objects W, X, Y, Z in $\mathbf{C}$:

$$\begin{array}{ccc} (X \otimes I) \otimes Y & \xrightarrow{\alpha_{X,I,Y}} & X \otimes (I \otimes Y) \\ & {\scriptstyle r_X \otimes \mathrm{id}_Y} \searrow \quad \swarrow {\scriptstyle \mathrm{id}_X \otimes l_Y} & \\ & X \otimes Y, & \end{array} \tag{C.1}$$

$$\begin{array}{ccccc} ((W \otimes X) \otimes Y) \otimes Z & \xrightarrow{\alpha_{W \otimes X,Y,Z}} & (W \otimes X) \otimes (Y \otimes Z) & \xrightarrow{\alpha_{W,X,Y \otimes Z}} & W \otimes (X \otimes (Y \otimes Z)) \\ {\scriptstyle \alpha_{W,X,Y} \otimes \mathrm{id}_Z} \downarrow & & & & \uparrow {\scriptstyle \mathrm{id}_W \otimes \alpha_{X,Y,Z}} \\ (W \otimes (X \otimes Y)) \otimes Z & & \xrightarrow{\alpha_{W,X \otimes Y,Z}} & & W \otimes ((X \otimes Y) \otimes Z). \end{array} \tag{C.2}$$

A symmetric monoidal category is a monoidal category with a natural isomorphism $b_{X,Y} : X \otimes Y \to Y \otimes X$ such that $b_{X,Y} \circ b_{Y,X} = \mathrm{id}_{Y \otimes X}$ and following diagrams commute for all objects X, Y, Z in $\mathbf{C}$:

$$\begin{array}{ccccc} X \otimes (Y \otimes Z) & \xrightarrow{\alpha^{-1}_{X,Y,Z}} & (X \otimes Y) \otimes Z & \xrightarrow{b_{X,Y} \otimes \mathrm{id}_Z} & (Y \otimes X) \otimes Z \\ {\scriptstyle b_{X,Y \otimes Z}} \downarrow & & & & \downarrow {\scriptstyle \alpha_{X,Y,Z}} \\ (Y \otimes Z) \otimes X & \xleftarrow[\alpha^{-1}_{Y,Z,X}]{} & Y \otimes (Z \otimes X) & \xleftarrow[\mathrm{id}_X \otimes b_{X,Z}]{} & Y \otimes (X \otimes Z), \end{array} \tag{C.3}$$

$$\begin{array}{ccccc} (X \otimes Y) \otimes Z & \xrightarrow{\alpha_{X,Y,Z}} & X \otimes (Y \otimes Z) & \xrightarrow{\mathrm{id}_X \otimes b_{Y,Z}} & X \otimes (Z \otimes Y) \\ {\scriptstyle b_{X \otimes Y,Z}} \downarrow & & & & \downarrow {\scriptstyle \alpha^{-1}_{X,Z,Y}} \\ Z \otimes (X \otimes Y) & \xleftarrow[\alpha_{Z,X,Y}]{} & (Z \otimes X) \otimes Y & \xleftarrow[b_{X,Z} \otimes \mathrm{id}_Y]{} & (X \otimes Z) \otimes Y. \end{array} \tag{C.4}$$

The associator enables us to regard $(X \otimes Y) \otimes Z$ and $X \otimes (Y \otimes Z)$ equal objects up to isomorphism in monoidal category. We can omit the parenthesis in the case the action of associator can be neglected, or when we assume the equivalence relation provided by the associator.

Among symemtric monoidal categories, cartesian categories are those whose tensor product is defined by the cartesian product.

Definition 46. A *cartesian category* is a category with the terminal object and cartesian products of arbitrary pairs of objects. When we regard a cartesian category as a symmetric monoidal category, its tensor product is defined by the cartesian product $X \times Y$ for objects. For morphisms, the tensor product $f \times g : X \times X' \to Y \times Y'$ of $f : X \to Y$ and $g : X' \to Y'$ is defined to be $\langle f \circ \pi_X, g \circ \pi_{X'} \rangle$, where $X \xleftarrow{\pi_X} X \times X' \xrightarrow{\pi_{X'}} X'$ are projectors. The unit is defined to be the terminal object.

By definition, product morphism $f \times g$ is the unique one that makes following diagram commute:

$$\begin{array}{ccccc} X & \xleftarrow{\pi_X} & X \times X' & \xrightarrow{\pi_{X'}} & X' \\ \downarrow{\scriptstyle f} & & \downarrow{\scriptstyle f\times g} & & \downarrow{\scriptstyle g} \\ Y & \xleftarrow{\pi_Y} & Y \times Y' & \xrightarrow{\pi_{Y'}} & Y.' \end{array} \tag{C.5}$$

C.3 Locales

In this section, we give definitions of locales for completeness. Chapters 5 and 6 are understandable from only the properties of the category of locales presented in the main text, without the precise definitions of locales given here. See, e.g. [41], for a more detailed introduction.

A poset L is called a *complete lattice* if it has joins and meets for all subsets of L. An element $x \in L$ is the join (meet) of subset S of L if $x \leq (\geq) y$ $(\forall y \in S)$ and if $z \leq (\geq) y$ $(\forall y \in S)$ implies $z \leq (\geq) x$. We denote the join (meet) of subset S by $\vee S$ $(\wedge S)$. In particular, $x \vee y$ and $x \wedge y$ represent the binary join $\vee\{x, y\}$ and meet $\wedge\{x, y\}$, respectively. We denote the top and the bottom element of the lattice by $\top$ and $\perp$, respectively.

If a complete lattice L further satisfies the infinite distributive law

$$x \wedge \bigvee S = \bigvee \{x \wedge y \mid y \in S\},$$

for any element $x \in L$ and any subset $S \subset L$, it is called a *locale* and also a *frame*. The difference between frame and locale only appears when we consider categories. Category **Frm** of frames has complete lattices with the infinite distributive law as objects, and functions $f^* : M \to L$ satisfying

$$\begin{aligned} f^*(\bigwedge S) &= \bigwedge \{f^*(x) \mid x \in S\} & (\forall S : \text{finite subset of } M), \\ f^*(\bigvee S) &= \bigvee \{f^*(x) \mid x \in S\} & (\forall S : \text{subset of } M), \end{aligned}$$

as morphisms from M to L. The objects of **Frm** are called frames. Category **Loc** of locales is the dual category of **Frm**, whose objects are now called locales. If $f : L \to M$ is a morphism in **Loc**, its dual morphism in **Frm** is denoted by $f^* : M \to L$. The morphisms in **Loc** are called continuous functions. They generalises continuous functions between topological spaces into pointless topology.

A locale L is further said to be compact if for any subset $S \subset L$ satisfying $\top = \bigvee S$, there is a finite element subset $S' \subset S$ such that $\top = \bigvee S'$. Define a binary relation $\leqslant$ on locale L by

$$x \leqslant y \text{ iff } \exists z \in L \text{ such that } x \wedge z = \perp, y \vee z = \top. \tag{C.6}$$

Locale L is said to be regular if

$$x = \bigvee \{y \in L \mid y \leqslant x\} \tag{C.7}$$

holds for any $x \in L$. The category **KRegLoc** of compact regular locales has compact regular locales as objects and continuous functions as morphisms.

The definition of completely regular locale is slightly more complicated. Define a binary relation $\preccurlyeq$ on locale L by $x \preccurlyeq y$ if there exists a sequence $\{z_q \mid q \in \mathbb{Q} \cap [0,1]\}$ of elements satisfying $x \leq z_0$, $z_1 \leq y$, and $z_p \leqslant z_q$ whenever $p \leq q$. Locale L is said to be completely regular if

$$x = \bigvee \{y \in L \mid y \preccurlyeq x\}, \tag{C.8}$$

holds for any $x \in L$. The category **KCRegLoc** of compact, completely regular locales has compact, completely regular locales as objects and continuous functions as morphisms.

C.4 Topos

This section gives an introduction to topos theory required for understanding of Chap. 5 and Chap. 6. In addition to a general topos theory, several properties of specific toposes appearing in our composite systems are reviewed. See e.g. [94] for more details on general topos theory.

An elementary topos is a certain category that satisfies several conditions.

Definition 47 (elementary topos)**.** A topos $\mathbf{T}$ is a category with all finite products and equalisers, equipped with an object Ω, with a function P which assigns to each object B an object PB, and, for each object A, with two isomorphisms, each natural in A,

$$\mathrm{Sub}_{\mathbf{T}}(A) \cong \mathrm{Hom}_T(A, \Omega), \tag{C.9}$$

$$\mathrm{Hom}_{\mathbf{T}}(B \times A, \Omega) \cong \mathrm{Hom}_{\mathbf{T}}(A, PB). \tag{C.10}$$

The object Ω is known to be the sub-object classifier of topos $\mathbf{T}$.

In topos **Sets**, the elements of set X of **Sets** are presented by morphisms of the form $1 \to X$ where $1 \cong \{*\}$ is the terminal object in **Sets**. In general topos, elements of object X refers to any morphisms with codomain X.

A *presheaf topos* is an example of topos that is used in the contravariant approach for topos quantum theory [89]. Contravariant functors from a category $\mathbf{C}$ to **Sets** are called presheaves over $\mathbf{C}$. A presheaf topos over $\mathbf{C}$ is $[\mathbf{C}^{op}, \mathbf{Sets}]$, which has presheaves over $\mathbf{C}$ as objects and natural transformations between them as morphisms.

The Bohrification approach and our generalisation to multipartite systems use functor category $[P, \mathbf{Sets}]$ with a certain poset P. There is an another representation of this functor category as a restriction of presheaf topos. We review this fact in the following subsection.

C.4.1 Sheaf topos

In this subsection, we give the definition of sheaf topos. The equivalence of functor category $[P, \mathbf{Sets}]$ with poset P and certain sheaf topos is shown. We use a particular kind of toposes $[P, \mathbf{Sets}]$ where P is given by the partial order of C*-algebras. The equivalence between $[P, \mathbf{Sets}]$ and sheaf toposes leads simple Kripke-Joyal semantics for $[P, \mathbf{Sets}]$ (see Appx. C.4.3).

A topological space X forms a category with its opens as objects and subset inclusion as morphisms ($U \to V \Leftrightarrow U \subset V$). If $t \in F(V)$ is an element of a set defined by a functor $F : \mathcal{O}(X)^{op} \to \mathbf{Sets}$ and if $U \subset V$ in $\mathcal{O}(X)$, we denote the element $F(f)(t)$ by $t|_U$, where $f : V \to U$ is the morphism in $\mathcal{O}(X)^{op}$.

Definition 48 (Sheaf)**.** A sheaf F on a topological space X is a presheaf F : $\mathcal{O}(X)^{op} \to \mathbf{Sets}$ such that for any $U \in \mathcal{O}(X)$ and its open covering $U = \cup_{i\in I} U_i$, the following diagram is an equaliser:

$$FU \xrightarrow{e} \prod_i FU_i \underset{q}{\overset{p}{\rightrightarrows}} \prod_{i,j} F(U_i \cap U_j), \tag{C.11}$$

where $e(t) = (t|_{U_1}, t|_{U_2}, ...)$ for $t \in FU$ and

$$\begin{aligned} & p(t_1, t_2, ...) \\ = \ & (t_1|_{U_1\cap U_1}, t_1|_{U_1\cap U_2}, ..., t_2|_{U_2\cap U_1}, t_2|_{U_2\cap U_2}, ..., ...), \end{aligned} \tag{C.12}$$

$$\begin{aligned} & q(t_1, t_2, ...) \\ = \ & (t_1|_{U_1\cap U_1}, t_2|_{U_1\cap U_2}, ..., t_1|_{U_2\cap U_1}, t_2|_{U_2\cap U_2}, ..., ...), \end{aligned} \tag{C.13}$$

for $(t_1, t_2, ...) \in \prod_i FU_i$.

The category *sheaf topos* on topological space X, denoted by $\mathrm{Sh}(X)$, has sheaves on X as objects and natural transformations between them as morphisms The definition of a sheaf implies that objects of $\mathrm{Sh}(X)$ are more restricted compared to those of presheaf topos $[\mathcal{O}(X)^{op}, \mathbf{Sets}]$.

Let us move onto a specific sheaves that is used later. Let $(P, \geq)$ be a poset. *Alexandrov topology* on a poset is a topology where open sets are upper sets of the order. Subset U of P is called an upper set if $x \in U$ and $x \leq y$ implies $y \in U$. For any element $x \in P$, subset $\uparrow x$ defined by

$$\uparrow x := \{y \in P | x \leq y\}, \tag{C.14}$$

is called a principle upper set. The correction of principle upper sets forms a base of the Alexandrov topology. The sheaf topos on poset P with the Alexandrov topology is denoted by $\mathrm{Sh}(P)$.

There is an isomorphism

$$\mathcal{I} : \mathrm{Sh}(P) \cong [P, \mathbf{Sets}]. \tag{C.15}$$

We show the invertible functor between $\mathrm{Sh}(P)$ and $[P, \mathbf{Sets}]$. Let us start from constructing a functor $\mathcal{I} : \mathrm{Sh}(P) \to [P, \mathbf{Sets}]$. The objects of $\mathrm{Sh}(P)$ are sheaves on P and those of $[P, \mathbf{Sets}]$ are functors from P to $\mathbf{Sets}$. Given a sheaf $F : \mathcal{O}(P) \to \mathbf{Sets}$, define a functor $\mathcal{I}(F) : P \to \mathbf{Sets}$ by

$$\mathcal{I}(F)(p) := F(\uparrow p), \tag{C.16}$$

$$\mathcal{I}(F)(p \leq q) := F(\uparrow q \subset \uparrow p) : F(\uparrow p) \xrightarrow{restriction} F(\uparrow q). \tag{C.17}$$

Based on the identification of arrow parts of the functors presented by Eq. (C.17), when we have an arrow $f : p \to q$ in the poset P (namely, $p \leq q$), and an element

$\alpha \in F(p)$ of a covariant functor $F : P \to \mathbf{Sets}$, we denote an element $F(f)(\alpha) \in F(q)$ by $\alpha|_q$. For an morphism in $\mathrm{Sh}(P)$, namely, a natural transformation $N : F \to G$ between sheaves, we define a natural transformation $\mathcal{I}(N) : \mathcal{I}(F) \to \mathcal{I}(G)$ by $\mathcal{I}(N)_p = N_{\uparrow p}$. Then the map $\mathcal{I} : \mathrm{Sh}(P) \to [P, \mathbf{Sets}]$ is a functor.

Next we make the inverse $\mathcal{I}^{-1} : [P, \mathbf{Sets}] \to \mathrm{Sh}(P)$. Given a functor $F : P \to \mathbf{Sets}$, define a functor $\mathcal{I}^{-1}(F) : \mathcal{O}(P)^{op} \to \mathbf{Sets}$ by

$$\begin{aligned} \mathcal{I}^{-1}(F)(U) &:= \cup_{i \in I} F(p_i) \text{ (where } U = \cup_{i \in I} \uparrow p_i)\text{(for upper sets)} \quad (C.18) \\ \mathcal{I}^{-1}(F)(U \subset V) &:= (F(V) \xrightarrow{restriction} F(U)) \text{ (for inclusion).} \end{aligned}$$

The definition of the functor for uppersets presented in Eq. (C.18) does not depend on which open covering for U is taken. For an morphism in $[P, \mathbf{Sets}]$, namely, a natural transformation $N : F \to G$ between functors, we define a natural transformation $\mathcal{I}^{-1}(N) : \mathcal{I}^{-1}(F) \to \mathcal{I}^{-1}(G)$ by $\mathcal{I}^{-1}(N)_U = \cup_{i \in I} N_{\uparrow p_i}$.

C.4.2 Mitchell-Bénabou language

In several points of the main text, we mentioned languages equipped to toposes, that enables interpretation of mathematical concepts. In this subsection, we give a superficial introduction to this language minimally required for proving several theorems presented in Chap. 5.

Most generally, mathematical sentences constitute of several formal symbols. Consider a statement

$$\forall r \in \mathbb{R}, (r^2 > 0 \Rightarrow r > 0) \quad (C.19)$$

for example. This statement can be decomposed into two statements $\phi_1(r) =$ "$r^2 > 0''$ and $\phi_2(r) =$ "$r > 0''$ which are both constructed from the variable $r \in \mathbb{R}$. They are first connected by *logical symbol* $\Rightarrow$ to form a larger term $\phi(r) =$ "$\phi_1(r) \Rightarrow \phi_2''$. Then logical symbol $\forall r \in \mathbb{R}$ turns $\phi(r)$ to a statement $\forall r \in \mathbb{R}, \phi(r)$ on which we may assign truth values ("*true*" or "$false$" in the case of set theoretic logic). Before considering the truth value of the statement (which is obviously false) in set theory, the usages of logical symbols $\Rightarrow$ and $\forall r \in \mathbb{R}$ to construct the sentence are already determined.

All the mathematical sentences constructed are called "terms". A term has its associated "type". There assumed to be a term called a "variable" for each type. There are rules for constructing terms by combining smaller terms with logical symbols such as $\wedge$, $\vee$, $\Rightarrow$, $\forall$, $\exists$. See [94] for more details. In the above example, $\mathbb{R}$ is a type and "r" is the variable of type $\mathbb{R}$.

There is a standard prescription to associate objects and morphisms of a topos for types and terms. Objects are associated to types. Identity morphism id_X of object X is associated to the variable of type X. General term of type X are morphisms whose codomain is X, and their domains are called sources. Terms of type Ω are called *formulas*. If a formula ϕ has variable x in its definition and if the variable is bounded neither by $\forall x$ nor by $\exists x$, the variable is said to be free. Action of logical symbols are represented by certain compositions of morphisms representing terms and logical symbols. See e.g. [94] for details. This association is called the interpretation of the logical symbols in the topos, and the resulting language written in terms of the objects and morphisms is called the Mitchell-Bénabou language internal to the topos. The Mitchell-Bénabou language internal to **Sets** coincides with the usual set-theoretic language.

Although we do not describe all the rules for the Mitchell-Bénabou language here, we review the role of the sub-object classifier Ω. When formula ϕ has free variables $x,\ y, ...$ of types $X,\ Y, ...$, it is constructed so that the source of ϕ is $X \times Y \times ...$, and we denote it by $\phi(x, y, ...) : X \times Y \times ... \to \Omega$. For an arbitrary topos and any formula $\phi(x) : X \to \Omega$, object $\{x|\phi(x)\}$ is defined to be the one that makes the following diagram a pullback:

$$\begin{array}{ccc} \{x|\phi(x)\} & \longrightarrow & 1 \\ \downarrow & & \downarrow{\scriptstyle \mathrm{true}} \\ X & \xrightarrow[\phi(x)]{} & \Omega, \end{array} \tag{C.20}$$

where true : $1 \to \Omega$ is the morphism making Ω the sub-object classifier. Roughly, the object $\{x|\phi(x)\}$ represents the collection of elements in X that satisfies $\phi(i)$. In topos **Sets**, Ω is the two value set $\{true,\ false\}$, and the morphism true is defined by true$(*) = true$. Then the set $\{x|\phi(x)\}$ is identical to

$$\{x' \in X|\phi(x)(x') = true\}, \tag{C.21}$$

where the parenthesis $\{\ |\ \}$ is defined by the usual set-theoretic way (conditioning). The definition given by (C.20) generalises the "subset of X whose elements satisfying $\phi(x)$" to the "sub-object of X whose elements satisfying $\phi(x)$".

A formula $\phi(x)$ with free variable x is said to be universally valid, if the sub-object $\{x|\phi(x)\}$ coincides with X itself. In particular if X is the terminal object 1, formulas with source 1 are said to hold if it is universally valid, and equivalently, if it coincides with true : $1 \to \Omega$. If $\phi(x)$ is a formula with source X, $\forall x\phi(x)$ is a formula with source 1. Formula $\phi(x)$ is universally valid if and only if $\forall x\phi(x)$ holds. We can easily imagine examples from **Sets**.

When there is a morphism $\alpha' : Y \to \{x|\phi(x)\}$ that makes diagram

$$\begin{array}{ccc} & & \{x|\phi(x)\} \\ & {\scriptstyle \alpha'}\nearrow & \downarrow \\ Y & \xrightarrow[\alpha]{} & X, \end{array}$$

commutes, then $\phi(x)$ is said to be valid for α and it is denoted by $Y \Vdash \phi(\alpha)$. In particular if $\phi : 1 \to \Omega$ does not have the free variable then $1 \Vdash \phi$ represents that ϕ holds.

C.4.3 Kripke-Joyal semantics

We use Kripke-Joyal semantics to decompose valid formulas into smaller formulas, in proving several theorems presented in Chap. 5. Kripke-Joyal semantics is a rule to turn logical symbols constituting formulas into the usual set-theoretical ones. For example,

$$Y \Vdash \phi_1(\alpha) \wedge \phi_2(\alpha) \text{ iff } Y \Vdash \phi_1(\alpha) \text{ and } Y \Vdash \phi_2(\alpha),$$

holds in any topos, where words "iff" and "and" (and "holds") in the sentence have usual set-theoretic meaning, while "$\wedge$" is defined by the Mitchell-Bénabou language. There are rules for turning other symbols to the set-theoretic ones.

Kripke-Joyal semantics takes an especially simple form on sheaf toposes where they are called sheaf semantics. Although sheaf semantics are defined on general Grothendieck toposes [94], we focus on the sheaf toposes over topological spaces.

For each open $U \in \mathcal{O}(X)$ of a topological space X, there exists a sheaf $\mathbf{s}U : \mathcal{O}(X)^{op} \to \mathbf{Sets}$ such that isomorphism

$$\mathrm{Hom}_{\mathrm{Sh}(X)}(\mathbf{s}U, A) \cong A(U), \tag{C.22}$$

holds for any sheaf $A : \mathcal{O}(X)^{op} \to \mathbf{Sets}$. Using this isomorphism, element $\alpha : \mathbf{s}U \to A$ is identified with an element $\alpha \in A(U)$ of a set. For the elements with these particular source, there exists an element $\alpha' : \mathbf{s}U \to \{a|\phi(a)\}$ that makes diagram

$$\begin{array}{ccc} & & \{a|\phi(a)\} \\ & \overset{\alpha'}{\nearrow} & \downarrow \\ \mathbf{s}U & \xrightarrow[\alpha]{} & A, \end{array} \tag{C.23}$$

commute, if and only if $\alpha \in \{a|\phi(a)\}(U)$ holds as an element of a set. Thus $\mathbf{s}U \Vdash \phi(\alpha)$ represents the commutativity of diagram (C.23) and equivalently $\alpha \in \{a|\phi(a)\}(U)$. We denote $\mathbf{s}U \Vdash \phi(\alpha)$ simply by $U \Vdash \phi(\alpha)$. In particular, the terminal object 1 of sheaf topos $\mathrm{Sh}(X)$ is presented by $\mathbf{s}X$. Thus $\phi : 1 \to \Omega$ holds if $X \Vdash \phi$.

The Kripke-Joyal semantics can be restricted to a decomposition rule on elements with sources $\mathbf{s}U$ with some open U, and the restricted version is called the sheaf semantics.

Theorem 49. [94] For a topological space X, let A be a sheaf on X, while $\phi(a)$ and $\psi(a)$ are formulas in the language of the sheaf topos $\mathrm{Sh}(X)$ over X and a is the free variable of type A; let $\alpha \in A(U)$. Then

(i) $U \Vdash \phi(\alpha) \wedge \psi(\alpha)$ iff $U \Vdash \phi(\alpha)$ and $U \Vdash \psi(\alpha)$;

(ii) $U \Vdash \phi(\alpha) \vee \psi(\alpha)$ iff there is a covering $\{U_i\}$ of U such that for each index i, either $U_i \Vdash \phi(\alpha|_{U_i})$ or $U_i \Vdash \psi(\alpha|_{U_i})$;

(iii) $U \Vdash \phi(\alpha) \Rightarrow \psi(\alpha)$ iff for all $V \subset U$, $V \Vdash \phi(\alpha|_V)$ implies $V \Vdash \psi(\alpha|_V)$;

Moreover, if $\phi(a, b)$ is a formula with free variables a of type A and b of type B, them for $\alpha \in A(U)$,

(iv) $U \Vdash \exists_b \phi(\alpha, b)$ iff there are a covering $\{U_i\}$ of U and elements $\beta_i \in B(U_i)$ such that $U_i \Vdash \phi(\alpha|_{U_i}, \beta_i)$ for each index i;

(v) $U \Vdash \forall_b \phi(\alpha, b)$ iff for all $V \subset U$ and all $\beta \in B(V)$, one has $V \Vdash \phi(\alpha|_V, \beta)$.

Sheaf toposes over posets with Alexandrov topology have a further simplified Kripke-Joyal semantics. In the right of isomorphism (C.15), we denote $\uparrow p \Vdash \phi(\alpha)$ by $p \Vdash \phi(\alpha)$ for principle uppersets $\uparrow p$ (seen as an open of $\mathcal{O}(P)$). Note that there are no coverings of principle uppersets other than the principle uppersets themselves for Alexandrov topology.

Theorem 50. For a poset P, let A be a covariant functor $A : P \to \mathbf{Sets}$, while $\phi(a)$ and $\psi(a)$ are formulas in the language of the topos $[P, \mathbf{Sets}] \cong \mathrm{Sh}(P)$ and a is the free variable of type A; let $\alpha \in A(p)$. Then

(i) $p \Vdash \phi(\alpha) \wedge \psi(\alpha)$ iff $p \Vdash \phi(\alpha)$ and $p \Vdash \psi(\alpha)$;

(ii) $p \Vdash \phi(\alpha) \vee \psi(\alpha)$ iff either $p \Vdash \phi(\alpha)$ or $p \Vdash \psi(\alpha)$;

(iii) $p \Vdash \phi(\alpha) \Rightarrow \psi(\alpha)$ iff for all $q \geq p$, $q \Vdash \phi(\alpha|_q)$ implies $q \Vdash \psi(\alpha|_q)$;

Moreover, if $\phi(a, b)$ is a formula with free variables a of type A and b of type B, then for $\alpha \in A(p)$,

(iv) $p \Vdash \exists_b \phi(\alpha, b)$ iff there is an element $\beta \in B(p)$ such that $p \Vdash \phi(\alpha, \beta)$;

(v) $p \Vdash \forall_b \phi(\alpha, b)$ iff for all $q \geq p$ and all $\beta \in B(q)$, one has $q \Vdash \phi(\alpha|_q, \beta)$.

We use this Kripke-Joyal semantics for obtaining the definitions of integrals internal to certain toposes.

C.4.4 Real numbers in $\mathrm{Sh}(P)$

In general toposes, definitions of natural numbers, rational numbers and real numbers differ from those in **Sets**. The real numbers object is constructed from the rational numbers object, which is constructed from natural numbers object whose existence is assumed by an axiom (called axiom of infinity). We do not follow the construction one by one here. A simple representation of the real number objects for sheaf toposes over topological spaces is already known.

Theorem 51. [94] The object $\mathbb{R}_{\mathrm{Sh}(X)} : \mathcal{O}(X)^{op} \to \mathbf{Sets}$ of (Dedekind) reals in the topos $\mathrm{Sh}(X)$ on a topological space X is (isomorphic to) the sheaf of continuous real-valued functions on the space X defined on the open sets W of X by

$$\mathbb{R}_{\mathrm{Sh}(X)}(W) = \{ f : W \to \mathbb{R} \mid f \text{ is continuous } \}. \tag{C.24}$$

If Thm. 51 is applied to topos $[P, \mathbf{Sets}]$ for poset P, we have

$$\mathbb{R}_{[P,\mathbf{Sets}]}(p) = \mathbb{R}_{\mathrm{Sh}(P)}(\uparrow p) = \{ f : \uparrow p \to \mathbb{R} \mid f \text{ is continuous } \}, \tag{C.25}$$

where the continuity is of course with respect to the Alexandrov topology. Since any Alexandrov continuous functions are constant, we obtain

$$\mathbb{R}_{[P,\mathbf{Sets}]}(p) = \{ f : \uparrow p \to \mathbb{R} \mid f \text{ is a constant function } \} \cong \mathbb{R}. \tag{C.26}$$

C.4.5 C*-algebras in $\mathrm{Sh}(P)$

C*-algebras are formally definable without referring to the actual toposes they are internalised. Here we review an already known form of internal C*-algebras in specific toposes, instead of tracking its formal definition. We use this simple expression for proving Thm. 23.

Internal C*-algebras have simple expressions for certain toposes.

Theorem 52. [109, Prop. 21] The object $\underline{A}$ (with additional structures $\underline{+}, \underline{\cdot}, \underline{*}, \underline{0}$) is a C*-algebra in the topos $[\mathbf{T}, \mathbf{Sets}]$ if and only if it is given by a functor $\underline{A} : \mathbf{T} \to \mathbf{Cstar}$, where **Cstar** is the category of C*-algebras and $*$-homomorphisms in **Sets**. The C*-algebra $\underline{A}$ is commutative if and only if each $\underline{A}(C)$ is commutative. The algebra $\underline{A}$ is unital if and only if every $\underline{A}(C)$ is unital and for each $f : C \to D$, the $*$-homomorphism $\underline{A}(f) : \underline{A}(C) \to \underline{A}(D)$ preserves the unit.

The additional structures $\underline{+}, \underline{\cdot}, \underline{*}$ are natural transformations representing summation, multiplication, and involution. A category is said to be small if both the collection of objects and morphisms are sets, and any poset P is small as a category. Thus we obtain the definition of internal commutative C*-algebras in $\mathrm{Sh}(P) \cong [P, \mathbf{Sets}]$ just by substituting P to $\mathbf{T}$ in Thm. 52.

Appendix D

Proofs for theorems in Chap. 5 and Chap. 6

D.1 Coproducts of internal unital commutative C*-algebras

This appendix shows Thm. 23 by generalising the method presented in Ref. [47]. We shall prove the following Lemma which directly implies the theorem:

Lemma 53. [95] Let P be a poset and functors $A_i : P \to \mathbf{Sets}$ $(i = 1, ..., n)$ be unital commutative C*-algebras internal to the functor topos $[P, \mathbf{Sets}]$. Then the object $A_1 \otimes ... \otimes A_n : P \to \mathbf{Sets}$ defined by

$$A_1 \otimes ... \otimes A_n(x) = A_1(x) \otimes ... \otimes A_n(x), \tag{D.1}$$

for elements (objects) $x \in P$ and

$$A_1 \otimes ... \otimes A_n(f)(a_1 \otimes ... \otimes a_n) = A_1(f)(a_1) \otimes ... \otimes A_n(f)(a_n), \qquad (a_i \in A_i(x)\ (\forall i)) \tag{D.2}$$

for partial orders (morphisms) $f : x \stackrel{\leq}{\to} y$, where the tensor products on the right hand sides of Eqs. (D.1) and (D.2) are for unital commutative C*-algebras in **Sets**, is an internal commutative C*-algebra. Furthermore it is the coproduct of $\{A_i\}_{i=1,...,n}$ in the category of internal unital commutative C*-algebras.

It is shown in Ref. [109] that an object A in $[\mathbf{T}, \mathbf{Sets}]$ is an internal unital commutative C*-algebra if and only if each component $A(x)$ is a unital commutative C*-algebra in **Sets** and the arrow part $A(f) : A(x) \to A(y)$ for any $f : x \to y$ in $\mathbf{T}$ is a unital *-homomorphism, where $\mathbf{T}$ is a small category (see Appx. C.4.5 for details). This implies that the object $A_1 \otimes \cdots \otimes A_n$ is an internal unital commutative C*-algebra, since each component $A_1 \otimes ... \otimes A_n(X)$ is a unital commutative C*-algebra in **Sets**, and a tensor product of unital *-homomorphisms is again a unital *-homomorphism. Note that poset P is a small category.

Interpretation of theories for unital *-homomorphisms by the Kripke-Joyal semantics on $[P, \mathbf{Sets}]$ reveals that a natural transformation $\alpha\colon A \to B$ between internal unital commutative C*-algebra objects A, B in $[P, \mathbf{Sets}]$ is an internal

*-homomorphism if and only if all the components are *-homomorphisms of unital commutative C*-algebras in **Sets**. For example, linearity

$$\forall a, b \in A, \alpha(a) + \alpha(b) = \alpha(a + b)$$

holds

$$\begin{array}{ll}
\text{iff} & \bot \Vdash \forall a, b \in A\colon \alpha(a) + \alpha(b) = \alpha(a+b), \\
\text{iff} & \forall p \in P,\ \forall a \in A(p),\ p \Vdash \forall b \in A\colon \alpha(a) + \alpha(b) = \alpha(a+b), \\
\text{iff} & \forall p \in P,\ \forall a \in A(p),\ \forall q \geq p,\ \forall b \in A(q),\ q \Vdash \alpha(a|_q) + \alpha(b) = \alpha(a|_q + b), \\
\text{iff} & \forall p \in P,\ \forall a \in A(p),\ \forall q \geq p,\ \forall b \in A(q),\ \alpha_q(a|_q) + \alpha_q(b) = \alpha_q(a|_q + b).
\end{array}$$

This statement is equivalent to the simpler statement

$$\forall p \in P,\ \forall a, b \in A(p),\ \alpha_p(a) + \alpha_p(b) = \alpha_p(a + b). \tag{D.3}$$

The other axioms for *-homomorphisms are interpreted similarly, and reduce to component-wise axioms in **Sets**.

Define natural transformations $\alpha^i\colon A_i \to A_1 \otimes \cdots \otimes A_n$ as the candidate coproduct injections by setting

$$\alpha^i_p(a_i) = \mathbb{I}_1 \otimes \cdots \otimes \mathbb{I}_{i-1} \otimes a_i \otimes \mathbb{I}_{i+1} \otimes \cdots \otimes \mathbb{I}_n. \tag{D.4}$$

These natural transformations are internal *-homomorphisms because each component is.

Now let A be any internal unital commutative C*-algebra, with internal *-homomorphisms $\beta^i\colon A_i \to A$. Consider morphisms $\gamma_p\colon A_1(p) \otimes \cdots \otimes A_n(p) \to A(p)$ defined for $p \in P$ by

$$\gamma_p(a_1 \otimes \cdots \otimes a_n) = \beta^1_p(a_1)\beta^2_p(a_2) \cdots \beta^n_p(a_n).$$

This is a natural transformation since for $f\colon p \to q$ we have

$$\begin{aligned}
&\gamma_q(A_1 \otimes \cdots \otimes A_n(f)(a_1 \otimes \cdots \otimes a_n)) \\
&= \gamma_q(A_1(f)(a_1) \otimes \cdots \otimes A_n(f)(a_n)) \\
&= \beta^1_y(A_1(f)(a_1))\beta^2_q(A_2(f)(a_2)) \cdots \beta^n_q(A_n(f)(a_n)) \\
&= A(f)(\beta^1_p(a_1))A(f)(\beta^2_p(a_2)) \cdots A(f)(\beta^n_p(a_n)) \\
&= A(f)(\beta^1_p(a_1)\beta^2_p(a_2) \cdots \beta^n_p(a_n)) \\
&= A(f)(\gamma_p(a_1 \otimes \cdots \otimes a_n)).
\end{aligned}$$

Clearly $\gamma \circ \beta^i = \alpha^i$ holds, and since each component is unique, γ is the unique mediating map satisfying this condition.

D.2 Internal integrals

We show that the internal integrals over $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$ is given by Def. 25, by interpreting the axioms for integrals by the Kripke-Joyal semantics [95].

Note first that the unit of multiplication $\mathbb{I}$ for $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$ is given by the component wise identities $\mathbb{I}_{C_1 \otimes \ldots \otimes C_n}$ $((C_1, ..., C_n) \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n))$, and the unit 1 of the internal real number object $\mathbb{R}$ is also given by the component wise unit. This implies that the normalisation condition $I(\mathbb{I}) = 1$ of the natural transformation $I : \underline{A_1} \otimes \cdots \otimes \underline{A_n} \to \mathbb{R}$ holds if and only if $I_C(\mathbb{I}_{C_1 \otimes \ldots \otimes C_n}) = 1$ for all $C_1 \otimes ... \otimes C_n \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n)$. Linearity and positivity are shown in the following manner.

Linearity of $I : \underline{A_1} \otimes \cdots \otimes \underline{A_n} \to \mathbb{R}$

$$\forall a, b \in \underline{A_1} \otimes \cdots \otimes \underline{A_n} \colon I(a) + I(b) = I(a + b)$$

holds

$$\begin{aligned}
&\text{iff} \quad \bot \Vdash \forall a, b \in \underline{A_1} \otimes \cdots \otimes \underline{A_n}, I(a) + I(b) = I(a + b), \\
&\text{iff} \quad \forall p \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n),\ \forall a \in \underline{A_1} \otimes \cdots \otimes \underline{A_n}(p),\ p \\
&\qquad \Vdash \forall b \in \underline{A_1} \otimes \cdots \otimes \underline{A_n} \colon I(a) + I(b) = I(a + b), \\
&\text{iff} \quad \forall p \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n),\ \forall a \in \underline{A_1} \otimes \cdots \otimes \underline{A_n}(p),\ \forall q \geq p, \\
&\qquad \forall b \in \underline{A_1} \otimes \cdots \otimes \underline{A_n}(q),\ q \Vdash I(a|_q) + I(b) = I(a|_q + b).
\end{aligned}$$

Under the representation of the internal real number $\mathbb{R}$ presented by Eq. (C.26), this statement is equivalent to

$$\begin{aligned}
&\forall p \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n),\ \forall a \in \underline{A_1} \otimes \cdots \otimes \underline{A_n}(p),\ \forall q \geq p, \\
&\forall b \in \underline{A_1} \otimes \cdots \otimes \underline{A_n}(q),\ I_q(a|_q) + I_q(b) = I_q(a|_q + b),
\end{aligned}$$

which is further equivalent to a simpler statement

$$\forall p \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n),\ \forall a, b \in \underline{A_1} \otimes \cdots \otimes \underline{A_n}(p),\ I_p(a) + I_p(b) = I_p(a + b).$$

Thus the natural transformation $I : \underline{A_1} \otimes \cdots \otimes \underline{A_n} \to \mathbb{R}$ is linear if and only if its components are all linear.

Positivity of $I : \underline{A_1} \otimes \cdots \otimes \underline{A_n} \to \mathbb{R}$

$$\forall a \in \underline{A_1} \otimes \cdots \otimes \underline{A_n} \colon a \geq 0 \Rightarrow I(a) \geq 0$$

holds

$$\begin{aligned}
&\text{iff} \quad \bot \Vdash \forall a \in \underline{A_1} \otimes \cdots \otimes \underline{A_n} \colon a \geq 0 \Rightarrow I(a) \geq 0, \\
&\text{iff} \quad \forall p \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n),\ \forall a \in \underline{A_1} \otimes \cdots \otimes \underline{A_n}(p),\ p \Vdash a \geq 0 \Rightarrow I(a) \geq 0, \\
&\text{iff} \quad \forall p \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n),\ \forall a \in \underline{A_1} \otimes \cdots \otimes \underline{A_n}(p),\ \forall q \geq p, \\
&\qquad q \Vdash a|_q \geq 0 \text{ implies } q \Vdash I(a|_q) \geq 0.
\end{aligned}$$

Under the representation of the internal real number $\mathbb{R}$ presented by Eq. (C.26), and the component-wise definition of internal C*-algebras presented by Thm. 52, this statement is equivalent to

$$\forall p \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n),\ \forall a \in \underline{A_1} \otimes \cdots \otimes \underline{A_n}(p),\ \forall q \geq p,\ a|_q \geq 0 \text{ implies } I_q(a|_q) \geq 0$$

which is further equivalent to a simpler statement

$$\forall p \in \mathcal{C}(A_1) \times \cdots \times \mathcal{C}(A_n),\ \forall a \in \underline{A_1} \otimes \cdots \otimes \underline{A_n}(p),\ a \geq 0 \text{ implies } I_p(a) \geq 0.$$

Thus the natural transformation $I : \underline{A_1} \otimes \cdots \otimes \underline{A_n} \to \mathbb{R}$ is positive if and only if its components are all positive.

In summary, a natural transformation $I : \underline{A_1} \otimes \cdots \otimes \underline{A_n} \to \mathbb{R}$ is an integral over $\underline{A_1} \otimes \cdots \otimes \underline{A_n}$ if and only if its components are all integrals in **Sets**. The naturality of I is equivalent to the lower condition in Def. 25.

D.3 Integrals and positive over pure tensor states

In this section, we present the proof of Theorem 26 which asserts the bijective correspondence between integrals and positive over pure tensor states [95]. We first introduce the notion of *unentangled frame functions*, and a generalisation of Gleason's theorem called the *unentangled Gleason's theorem*, which are required for the proof.

Functions which have values on unentangled bases of composite Hilbert spaces have been previously analysed under the name of *unentangled frame functions*. More precisely, they are defined as follows.

Definition 54 (unentangled frame function [110, 111])**.** Let H_i $(i = 1, ..., N)$ be Hilbert spaces, and $\mathrm{Prod}(H_1, ..., H_N)$ be the set of all product unit vectors on $H_1 \otimes ... \otimes H_N$. An unentangled frame function for $H_1, ..., H_N$ is a function $f : \mathrm{Prod}(H_1, ..., H_N) \to \mathbb{R}^+$ such that for some positive number w (called the weight of f), $\sum_j f(\xi_j) = w$ holds whenever $\{\xi_j\}_j$ is an orthonormal basis of $H_1 \otimes ... \otimes H_N$ with each $\xi_j \in \mathrm{Prod}(H_1, ..., H_N)$.

We denote the set of unit-weight unentangled frame functions for $H_1, ..., H_N$ by $\mathrm{UFF}^1(H_1, \ldots, H_n)$. The notion of unentangled frame function is an extension of the frame function defined in Ref. [45], where the correspondence between quantum states on a single system and frame functions on the system is shown. For composite systems, the following theorem is known.

Theorem 55. [111, Thm. 1] Let $H_1, ..., H_N$ be finite-dimensional Hilbert spaces of each dimension at least 3. Let $f : \mathrm{Prod}(H_1, ..., H_N) \to \mathbb{R}^+$ be an unentangled frame function. Then there exists a self-adjoint operator ω_f in $\mathcal{B}(\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n)$ such that whenever $v_1 \otimes ... \otimes v_N$ is in $\mathrm{Prod}(H_1, ..., H_N)$ and p_i is the projection of H_i onto the one-dimensional subspace generated by v_i,

$$f(v_1 \otimes ... \otimes v_n) = \mathrm{Tr}(p_1 \otimes ... \otimes p_n)\omega_f. \tag{D.5}$$

The uniqueness of ω_f for a given f in this Theorem is shown in Ref. [110], although it is not explicitly mentioned in Ref. [111].

Theorem 55 implies the bijective correspondence between positive over pure tensor states and unit-weight unentangled frame functions, and called "unentangled Gleason's theorem". Under this correspondence, Theorem 26 is rewritten in terms of the unentangled frame functions as follows: an injective map from $\mathrm{UFF}^1(H_1, \ldots, H_n)$ to integrals defined by

$$f \mapsto \{I^f_{(C_1,\ldots,C_N)} : (C_1 \otimes \ldots \otimes C_N)_{sa} \to \mathbb{R}\}_{(C_1,\ldots,C_N)\in\mathcal{C}(A_1)\times\cdots\times\mathcal{C}(A_n)}, \tag{D.6}$$

$$I^f_{(C_1,\ldots,C_N)}(p_1 \otimes \ldots \otimes p_N) = f(v_1 \otimes \ldots \otimes v_n) \qquad (\text{if } p_i \in C_i \text{ for all } i), \tag{D.7}$$

where p_i is the projector onto the one-dimensional subspace generated by v_i, is a bijection if the dimension of all the Hilbert spaces H_i is at least 3.

We show that a map from integrals to $\mathrm{UFF}^1(H_1, \ldots, H_n)$ presented by

$$\{I_{(C_1,\ldots,C_N)} : (C_1\otimes, \ldots, \otimes C_N)_{sa} \to \mathbb{R}\}_{(C_1,\ldots,C_N)\in\mathcal{C}(A_1)\times\cdots\times\mathcal{C}(A_n)} \mapsto f^I, \tag{D.8}$$

$$f^I(v_1 \otimes \ldots \otimes v_n) = I_{(C_1,\ldots,C_N)}(p_1 \otimes \ldots \otimes p_N) \qquad (\text{if } p_i \in C_i \text{ for all } i), \tag{D.9}$$

is well-defined and injective. First observe for any internal integral $\{I_{(C_1,\ldots,C_N)}\}_{(C_1,\ldots,C_N)\in\mathcal{C}(A_1)\times\cdots\times\mathcal{C}(A_n)}$, and for all product projectors $p_1 \otimes \ldots \otimes p_N \in (C_1\otimes, \ldots, \otimes C_N)_{sa} \cap (C'_1\otimes, \ldots, \otimes C'_N)_{sa}$, we have

$$\begin{aligned} I_{(C_1,\ldots,C_N)}(p_1 \otimes \ldots \otimes p_N) &= I_{(C_1\cap C'_1,\ldots,C_N\cap C'_N)}(p_1 \otimes \ldots \otimes p_N) \\ &= I_{(C'_1,\ldots,C'_N)}(p_1 \otimes \ldots \otimes p_N), \end{aligned}$$

since $p_1 \otimes \ldots \otimes p_N \in (C_1\otimes, \ldots, \otimes C_N)_{sa} \cap (C'_1\otimes, \ldots, \otimes C'_N)_{sa}$ implies $p_1 \otimes \ldots \otimes p_N \in (C_1 \cap C'_1 \otimes \ldots \otimes C_N \cap C'_N)_{sa}$. Thus the value of integration does not depend on the context, and the map presented by Eq. (D.9) is well-defined. Furthermore, the map is injective, since the context-wise linearity of integrals reveals that an integral is uniquely determined by its value on product projectors.

The map defined by Eq. (D.9) is the inverse of the map defined by Eq. (D.7). This completes the proof of Theorem 26.

D.4 Proof of Lem. 31

We prove Lem. 31 [95]. If we represent the Kleisli composition in the left hand side of Eq. (6.5) by the usual composition in $\mathbf{C}$, the left hand side is transformed to the right hand side via

$$\begin{aligned} & \mu_{X'\times Y'} \circ T(i_{X'\times Y'} \circ (f \times g)) \circ i_{X,Y} \circ \langle p_X,\ p_Y\rangle & \text{(D.10)} \\ = \ & \mu_{X'\times Y'} \circ Ti_{X'\times Y'} \circ T(f \times g) \circ i_{X,Y} \circ \langle p_X,\ p_Y\rangle & \text{(D.11)} \\ = \ & \mu_{X'\times Y'} \circ Ti_{X'\times Y'} \circ i_{TX,TY} \circ (Tf \times Tg) \circ \langle p_X,\ p_Y\rangle, & \text{(D.12)} \\ = \ & i_{X'\times Y'} \circ (\mu_{X'} \times \mu_{Y'}) \circ (Tf \times Tg) \circ \langle p_X,\ p_Y\rangle & \text{(D.13)} \\ = \ & i_{X'\times Y'} \circ \langle f \odot p_X, g \odot p_Y\rangle. & \text{(D.14)} \end{aligned}$$

Here, the second equality comes from the naturality of i. The third equality comes from the commutativity of

$$\begin{array}{ccccc} T^2X \otimes T^2Y & \xrightarrow{i_{TX,TY}} & T(TX \otimes TY) & \xrightarrow{Ti_{X,Y}} & T^2(A \otimes B) \\ \Big\downarrow{\scriptstyle \mu_A\otimes\mu_B} & & & & \Big\downarrow{\scriptstyle \mu_{X\otimes Y}} \\ TX \otimes TY & & \xrightarrow{\quad i_{X,Y} \quad} & & T(X \otimes Y), \end{array}$$

for any pair of X and Y, which is shown for any commutative monad on symmetric monoidal categories in Ref. [102].

D.5 Proof of Lem. 32

In this section, we prove Lem. 32 [95]. The left hand side of Eq. (6.9) is transformed into

$$T\pi_{Y\times Z} \circ \mu_{X\times Y\times Z} \circ T\mathrm{ext} \circ p = \mu_{Y\times Z} \circ T^2\pi_{Y\times Z} \circ T\mathrm{ext} \circ p \tag{D.15}$$
$$= \mu_{Y\times Z} \circ T(T\pi_{Y\times Z} \circ \mathrm{ext}) \circ p, \tag{D.16}$$

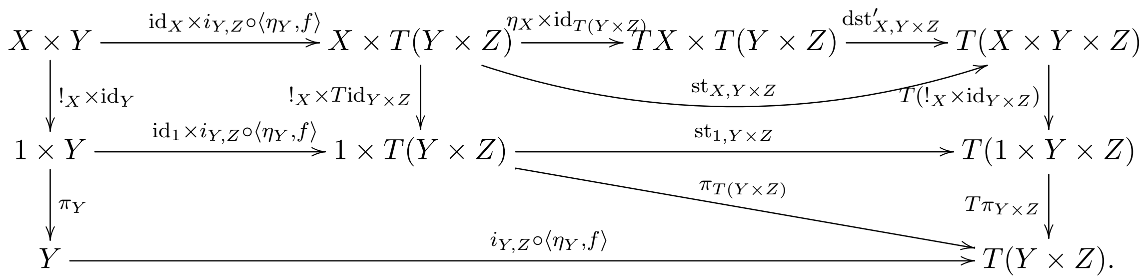
where the first equality comes from the naturality of μ. The right hand side of Eq. (6.9) is transformed into

$$\mu_{Y\times Z} \circ T(i_{Y,Z} \circ \langle \eta_X, f\rangle) \circ T\pi_Y \circ p = \mu_{Y\times Z} \circ T(i_{Y,Z} \circ \langle \eta_X, f\rangle \circ \pi_Y) \circ p. \tag{D.17}$$

Thus Eq. (6.9) holds if

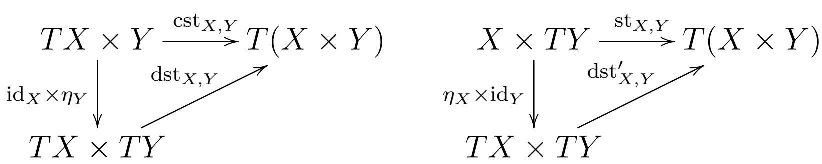
$$T\pi_{Y\times Z} \circ \mathrm{ext} = i_{Y,Z} \circ \langle \eta_X, f\rangle \circ \pi_Y. \tag{D.18}$$

Although $\mathrm{dst} = \mathrm{dst}' = i$ for commutative monads, it is convenient to substitute dst' to i for a moment. Consider the following diagram:



The compositions of arrows from $X \times Y$ to $T(X \times Y)$, going lower-left edges and upper-right edges represent the right and left hand sides of Eq. (D.18). The left two squares commute by the definition of product, the lower right triangle by the condition (1.27) for the strength, the right square by the naturality of strength, and the upper right triangle by Lem. 56 shown below. Thus all the triangles and squares commute and we have shown Eq. (D.18) when i is dst'.

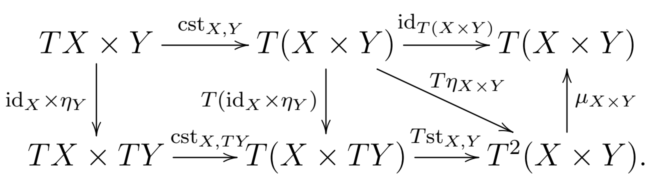
Lemma 56. [112] Triangles



(D.19)

commute.

Proof. Although the commutativity of these diagrams is suggested in Ref. [112], we provide an explicit proof since we were unable to find it in the literature. By decomposing dst according to its definition, the left triangle decomposes into



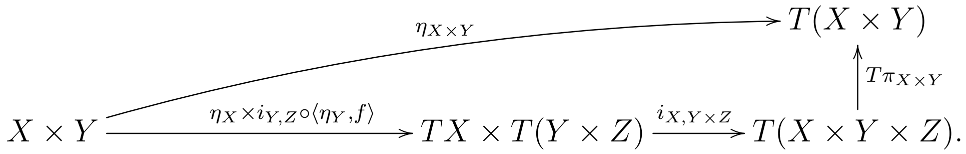
The left square commutes by the naturality of cst, the lower triangle by the unit law of strength (the upper triangle of (1.29)), and the upper triangle is the unit law of monad. The commutativity of the right triangle can be shown by a symmetric argument. $\square$

D.6 Proof of Lem. 33

In this section, we give a proof of Lem. 33 [95]. Equation (6.11) is rewritten into

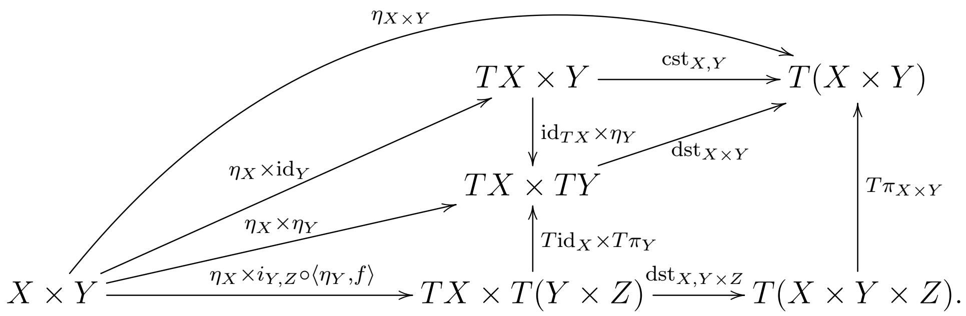
$$p = T\pi_{X\times Y} \circ \mu_{X\times Y\times Z} \circ T\mathrm{ext} \circ p \;=\; \mu_{X\times Y} \circ T^2\pi_{X\times Y} \circ T\mathrm{ext} \circ p, \quad \text{(D.20)}$$
$$= \mu_{X\times Y} \circ T(T\pi_{X\times Y} \circ \mathrm{ext}) \circ p, \quad \text{(D.21)}$$

where the second equality comes from the naturality of μ. This holds if $T\pi_{X\times Y} \circ \mathrm{ext} = \eta_{X\times Y}$, in other words, if the following diagram commute:



(D.22)

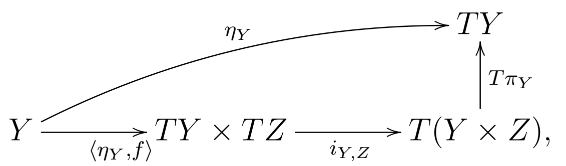
Although $i = \mathrm{dst} = \mathrm{dst}'$ holds for commutative monad, it is convenient to substitute $i = \mathrm{dst}$ for a moment. Consider following decomposition of diagram (D.22) into pieces

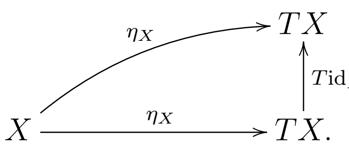


(D.23)

The triangle at the top represents the unit law for cst (the upper triangle of diagram (1.29)). The centre left triangle is trivial. The square commutes from the naturality of dst, because $T\pi_{X\times Y} = T(\mathrm{id}_X \times Y)$. The centre right triangle is in Lem. 56. The lower left triangle is the only one whose commutativity is not shown.

By the definition of product $\times$, the lower left triangle decomposes into two triangles





The right triangle clearly commutes. Thus diagram (D.22) commutes if the left triangle commutes, which is guaranteed by Lem. 57 shown below. This completes the proof.

Lemma 57. [95] If $T1 \cong 1$ for a strong monad (T, η, μ) on a cartesian category, the following diagrams commute:

$$\begin{array}{ccc} & & TX \\ & \overset{\pi_{TX}}{\nearrow} & \uparrow{\scriptstyle T\pi_X} \\ TX \times TY & \xrightarrow[\mathrm{dst}_{X,Y}]{} & T(X \times Y), \end{array} \qquad \begin{array}{ccc} TX \times TY & \xrightarrow{\mathrm{dst}'_{X,Y}} & T(X \times Y) \\ & \underset{\pi_{TY}}{\searrow} & \downarrow{\scriptstyle T\pi_Y} \\ & & TY, \end{array} \tag{D.24}$$

for any objects X and Y.

Proof. This lemma is already known for cartesian *closed* categories [112]. We here extend this known result on cartesian closed categories into cartesian categories not necessary closed. We prove the left triangle, writing $! : Y \to 1$. Note that projection $\pi_X : X \times Y \to X$ can be decomposed into $X \times Y \xrightarrow{\mathrm{id}_X \times !} X \times 1 \xrightarrow{\pi_X} X$. It follows from naturality of dst that

$$\begin{aligned} &T\pi_X \circ \mathrm{dst}_{X,Y} = T(\pi_X \circ \mathrm{id}_X \times !) \circ \mathrm{dst}_{X,Y} \\ &= T\pi_X \circ \mathrm{dst}_{X,1} \circ T\mathrm{id}_X \times T! = T\pi_X \circ \mathrm{dst}_{X,1} \circ \mathrm{id}_{TX} \times T!, \end{aligned}$$

so it suffices to show $T\pi_X \circ \mathrm{dst}_{X,1} = \pi_{TX}$. But this follows from the proof of [112, Thm. 2.1]; notice that while that result assumes cartesian closedness, only cartesianness is sufficient for our purpose. The right triangle of (D.24) can be shown by a symmetric argument. □

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