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博士論文

Quantum algorithms for higher-order quantum transformations of universal unitary operations

（普遍的なユニタリ操作に対する高階量子変換の
量子アルゴリズム）

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Abstract

Higher-order quantum transformations describe transformations between quantum operations. Higher-order quantum transformations are used for analyzing the properties of quantum operations, and are expected to bring further insights to quantum mechanics. In quantum algorithms, computational tasks are usually encoded as quantum operations, and a physical realization of higher-order quantum transformations is expected to provide a comprehensive implementation of those quantum algorithms. In this thesis, we focus on higher-order quantum transformations on unitary operations, as many quantum algorithms can be described by unitary operations, and general quantum operations can be represented by unitary operations acting on an extended quantum system.

The first topic we focus on is *quantum switch*, a higher-order quantum transformation used for the study of the causal structure of quantum operations within quantum mechanics. We investigate the difference between the action of quantum switch on unitary operations and that on general quantum operations beyond unitary operations, and we show that they coincide under certain natural assumptions. This result strengthens the theoretical background for the studies on quantum switch, and provides a physical meaning to the experimental realization of quantum switch.

The second topic is *controllization*, a higher-order quantum transformation from a unitary operation to the corresponding controlled unitary operation. It is a quantum counterpart of the "if-clause" in classical computing. We extend the definition of controlled unitary operations to controlled general quantum operations and further to controlled higher-order quantum transformations. We analyze controllization as a controlled version of a certain class of higher-order quantum transformations, and propose a new quantum algorithm for approximate controllization without using an auxiliary system.

In the last topic, we propose a new structure of higher-order quantum transformation named *success-or-draw*, which allows a repeat-until-success strategy. The repeat-until-success strategy allows an exponentially decreasing failure probability for probabilistic algorithms. However, in probabilistic higher-order quantum transformations, the initial input state cannot be re-used on failure, and the applicability of a repeat-until-success strategy is not straightforward. We mathematically identify a structure that allows re-use of the initial input state on failure as the success-or-draw structure, and we prove that this structure is compatible with a large class of higher-order quantum transformations. We also analyze a higher-order quantum transformation known as unitary inversion in terms of success-or-draw, and propose a protocol with a higher success probability than previously known ones.

List of Publications

This thesis is based on the following papers.

1. Q. Dong, S. Nakayama, A. Soeda, and M. Murao, "Controlled quantum operations and combs, and their applications to universal controllization of divisible unitary operations," `arXiv:1911.01645 [quant-ph]`.

2. Q. Dong, M. T. Quintino, A. Soeda, and M. Murao, "Success-or-draw: A strategy allowing repeat-until-success in quantum computation," `arXiv:2011.01055 [quant-ph]`.

This thesis also uses the results in the following previous works of the author.

3. Q. Dong, M. T. Quintino, A. Soeda, and M. Murao, "Implementing positive maps with multiple copies of an input state," *Phys. Rev. A* **99** (May, 2019) 052352, `arXiv:1808.05788 [quant-ph]`.

4. M. T. Quintino, Q. Dong, A. Shimbo, A. Soeda, and M. Murao, "Reversing unknown quantum transformations: A universal quantum circuit for inverting general unitary operations," *Phys. Rev. Lett.* **123** (Nov, 2019) 210502, `arXiv:1810.06944 [quant-ph]`.

5. M. T. Quintino, Q. Dong, A. Shimbo, A. Soeda, and M. Murao, "Probabilistic exact universal quantum circuits for transforming unitary operations," *Phys. Rev. A* **100** (Dec, 2019) 062339, `arXiv:1909.01366 [quant-ph]`.

Contents

Notations

- $\mathcal{H}, \mathcal{I}, \mathcal{O}$: Hilbert spaces.
- $\mathcal{L}(\mathcal{H})$: The set of linear operators on $\mathcal{H}$.
- $|\psi\rangle^{\mathcal{H}}, \rho^{\mathcal{H}}$: Quantum states in the Hilbert space $\mathcal{H}$.
- δ_{ij}: The Kronecker delta.
- $\widetilde{id}$: The identity operation.
- $|U\rangle\rangle$: The unnormalized maximally entangled state defined by $(I \otimes U)|I\rangle\rangle := \sum_i |i\rangle(U|i\rangle)$
- J_U: The Choi operator of unitary operation U defined by $J_U := |U\rangle\rangle\langle\langle U|$.
- $\widetilde{\widetilde{\mathcal{A}}}$: A supermap.
- $\widetilde{\mathcal{A}}$: The corresponding map of the supermap $\widetilde{\widetilde{\mathcal{A}}}$, or a quantum operation.
- A: The Choi operator of the supermap $\widetilde{\widetilde{\mathcal{A}}}$.

Chapter 1

Introduction

1.1 Quantum Information Processing

Quantum mechanics presents various new phenomena not exhibited in classical mechanics such as quantum entanglement. Quantum mechanics provides a new understanding of the fundamental principles of our world, and new technologies not achievable within classical mechanics. Quantum information processing [1–4] is one of the emerging technologies utilizing various unique phenomena of quantum mechanics for information processing. Some information processing tasks can be more efficiently performed in quantum mechanics than in classical mechanics. One of the most famous tasks is factoring, which can be solved in a polynomial time using a quantum algorithm, Shor's algorithm [5], and is considered to have an exponential speed-up by utilizing properties of quantum mechanics. Quantum key distribution [6] also provides secure communication with quantum mechanics.

While developing technologies for utilizing unique properties of quantum mechanics is inevitable for performing quantum information processing, discovering novel quantum algorithms including Shor's algorithm remains an active field of research. Quantum mechanics introduces many operations for information processing not existing in classical mechanics such as creating a superposition of states, but it also forbids many intuitive operations used in classical information processing such as cloning of unknown quantum states [7]. Thus, it is important to clarify which operations are possible within quantum mechanics.

There exist various models for quantum computing including the quantum circuit model, measurement-based quantum computation [8, 9], and adiabatic quantum computation [10]. The quantum circuit model is widely used because it intuitively describes information processing tasks corresponding to the classical counterpart. In the quantum circuit model, input data for information

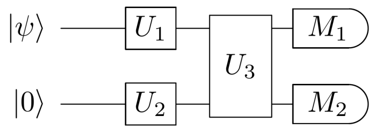


Figure 1.1: An example of a quantum circuit. The input state is $|\psi\rangle$ and a fixed auxiliary state $|0\rangle$. Unitary operations U_1, U_2, and U_3 are applied on the quantum states in order, and quantum measurements M_1, M_2 give outcomes represented by classical information. Each horizontal line presents a quantum system, and the operations are applied from left to right.

processing tasks are usually encoded in quantum states, and the "program" is described by a sequence of quantum operations as shown in Fig. 1.1.

The quantum circuit model describes quantum algorithms in an abstract way, in the sense that transformations of quantum states are not described by the actual time evolution generated by a Hamiltonian of the quantum system constituting a quantum computer. Quantum algorithms are described by a sequence of elemental operations in the quantum circuit model. The basic building blocks of the quantum circuit model are the quantum gates, usually a finite set of unitary operations and quantum measurements in a certain basis often fixed in a basis called the computational basis. In many quantum algorithms, a sequence of unitary operations is applied, and quantum measurements are performed in the last step to obtain outcomes given by classical information from the quantum states transformed by the sequence of unitary operations. For that, unitary operations are considered to be the most basic building block for quantum information processing.

1.2 Higher-order Quantum Operations

In spite of being widely used, describing quantum algorithms in terms of the quantum circuit model becomes complicated when the tasks become complex and the number of required quantum gates increases. Moreover, the developments of quantum technologies allow us to exploit larger quantum systems for performing such complex tasks. Thus, new methods for describing quantum algorithms are in demand for future developments in quantum information theory, and many attempts have been made recently. One of the recent developments is *higher-order quantum operations* [11, 12]. While usual quantum operations describe transformations between quantum states, higher-order quantum operations describe transformations between quantum operations.

Higher-order quantum operations can be regarded as the quantum counterpart of higher-order functions in many programming languages in classical computing, and are expected to provide an alternative way of quantum programming. Especially, in many computational tasks, the properties of the tasks are encoded as quantum operations, instead of quantum states, in various forms, and a physical realization of higher-order quantum operations are expected to provide a comprehensive implementation of quantum algorithms. Also, since quantum operations describe dynamics of quantum systems, higher-order quantum operations can be used for analyzing the transformability of quantum dynamics, and bring further insights to quantum mechanics.

In order to understand how higher-order quantum operations are used for quantum algorithms, here we introduce a few examples of higher-order quantum operations. The first example of higher-order quantum operation is *unitary inversion*: transforming a unitary operation into its inverse operation [13–17]. A schematic view of the problem is given in Fig. 1.2. Given a unitary operation, its inverse operation is also a unitary operation. If the unitary operation, or the corresponding unitary operator, is given by its classical description, such as a matrix with all elements known, obtaining the inverse operation is simple in principle, because the inverse of a unitary matrix can be calculated as the transposition and complex conjugation of the original matrix. However, if the unitary operation is given by a Hamiltonian dynamics, obtaining the inverse operation becomes a non-trivial task because it is not possible to invert the time evolution of a quantum system in general. Many quantum algorithms, for example the Harrow-Hassidim-Lloyd (HHL) algorithm [18] that solves a linear equation, use a unitary operation characterizing the problems and its inverse operation in pairs. If it is possible to universally invert a unitary operation without specifying its classical description, this kind of quantum algorithms can be realized more simply because once we construct a quantum circuit of the unitary operation characterizing the problems, its inverse operation can also be implemented by using the same unitary operation, and it is not necessary to construct another quantum circuit only for the inverse operation.

Another example of higher-order quantum operation is *controllization*: transforming a unitary operation into the corresponding controlled unitary operation [17, 19–25]. A controlled unitary operation is also a unitary operation and its action is given as follows: if the control system is in state $|0\rangle$, it applies the identity operation to the target system; if the control system is in state $|1\rangle$, it applies the corresponding unitary operation to the target system; and if the control

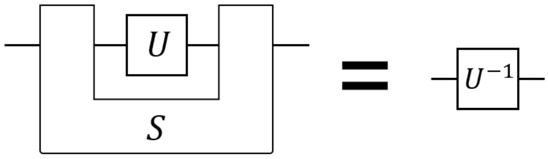


Figure 1.2: A schematic picture of an example of a higher-order quantum operation called unitary inversion. The higher-order quantum operation by a concave box denoted by S transforms a unitary operation U into its inverse U^{-1}. Many algorithms use U and U^{-1} in pairs. If this higher-order quantum operation is implementable, we can replace the use of U^{-1} with repetitive uses of U together with S, instead of implementing U^{-1} regardless of U.

system is in a superposition of $|0\rangle$ and $|1\rangle$, it applies the coherent superposition of the two operations. Controlled unitary operations are widely used in various quantum algorithms including Shor's algorithm for factoring, the HHL algorithm for solving linear equations, and Kitaev's phase estimation algorithm [26]. Controlled unitary operations are a quantum counterpart of the "if-operation" in classical computing, and similarly, controllization is a quantum counterpart of the "if-clause", which transforms an operation into an "if-operation", in classical computing. As the "if-clause" is a key element in classical computing, controllization is expected to be a useful higher-order quantum operation in quantum computing.

Higher-order quantum operations are also used for the study of the relationship between space and time in quantum information processing. A recent emerging topic in this category is the *indefinite causal order* [27–30]. Usual situations considered for higher-order quantum operation are to use the input operations in a fixed time order. However, if higher-order quantum operations are considered as just a transformation between quantum operations, there is no fundamental principle of quantum mechanics to rule out the possibility of using input operations in superposition, which is also known as the indefinite causal order. The simplest example of higher-order quantum operation with indefinite causal order is *quantum switch*: transforming a pair of unitary operations into a superposition of two differently ordered concatenations of the pair of input unitary operations [27]. Quantum switch is shown to be not implementable within the usual quantum circuit model, but no principle of quantum mechanics is found to forbid the implementation of quantum switch so far. Quantum switch is not just an academically interesting example of indefinite causal order, but it is shown to provide certain advantages in quantum computing and quantum communication tasks [31–36].

We have listed three examples of higher-order quantum operations and their importance in quantum physics and quantum information processing. There are other higher-order quantum operations that have been investigated, for example, cloning of unitary operation [37], store and retrieve of unitary operations [38,39]. A common feature of these useful higher-order quantum operations is that they are basically defined for unitary operations, that is, we usually focus on the action of higher-order quantum operations on unitary operations instead of general quantum operations. Unitary operations are one of the most fundamental quantum operations in quantum information processing, and in many quantum algorithms, tasks are encoded into unitary operations. As one of the main reasons to utilize higher-order quantum operation is to perform the tasks of quantum information processing, it is natural to focus on the action on unitary operations where the tasks are encoded. However, when we actually implement a higher-order quantum operation in a quantum circuit, for example, it is always possible to input general quantum operations instead of unitary operations as input operations. That is, even when we only consider the action of higher-order quantum operations on unitary operations, the action on general quantum operations must be determined in a certain manner.

1.3 Implementing Higher-order Quantum Operations

Higher-order quantum operations yield various applications if they are implemented. However, it is not obvious how these higher-order quantum operations can be implemented in quantum mechanics. A mathematical formulation of higher-order quantum operations that is compatible with the quantum circuit model [11, 12] provides a tool for analyzing what kind of higher-order quantum operations are implementable. Unfortunately, many of the higher-order quantum operations are shown to be not implemented in an exact and deterministic manner [16, 37, 38]. On the other hand, there are various attempts for implementing higher-order quantum operations by relaxing certain restrictions. For example, it is usually considered the case where multiple uses of input quantum operations are allowed. By such relaxations, there exists a universal way for approximately implementing higher-order quantum operations: first extract the classical description of the input operation, for example by utilizing quantum process tomography [40]; then calculate the output operation of the higher-order quantum operation in a classical way; and finally implement the corresponding output operation based on the calculated classical description. This method can be used to implement higher-order quantum operation with an arbitrarily small error if enough number of uses of the input operation is allowed. However, this method does not provide many advantages of higher-order quantum operation, because the calculation of higher-order quantum operation is mainly performed in a classical way. Also, this method does not implement the exact higher-order quantum operation, because quantum process tomography cannot provide exact classical description with a finite number of uses of the input operation.

In this thesis, we focus on the properties of three types of higher-order quantum operations. Apart from its concrete formalism, finding out how to implement higher-order quantum operation is still a hard problem in general due to the exponential nature of the Hilbert space to be analyzed. Thus, we focus on the analysis of certain types of higher-order quantum operations, especially those on unitary operations, and provide new understandings of the possibilities and limitations of higher-order quantum operations. We also propose new quantum algorithms for efficient implementations of certain higher-order quantum operations, and provide new methods for the experimental realization of higher-order quantum operations.

Quantum Switch The first topic we focus on is quantum switch. Quantum switch is a well-studied higher-order quantum operation as we stated, but its definition has not been concrete in the following sense: when the two input operations are unitary operations, the output operation is given by coherently controlled two differently causally ordered operations; however, when two input operations are not unitary operations, the output operation cannot be simply extended as a coherent superposition as in the unitary case. In the definition of quantum switch [27], the action on general quantum operations is chosen to be the most natural one based on its Kraus representation [41]. This definition is widely used in various studies of quantum switch on general quantum operations [33–36], but it has not been known if this definition is the only possible definition compatible with its action on unitary operations.

In this thesis, we show that the action of quantum switch on general quantum operations can be uniquely determined from its action on unitary operations by adding two natural assumptions. Moreover, if either of the two assumptions is omitted, the uniqueness does not hold. This result strengthens the theoretical background for the studies on quantum switch, and provides a physical meaning to the experimental realization of quantum switch because the assumptions we pose are necessary to promise the action of quantum switch on general quantum operations.

Controllization The second topic is controllization. Controllization has been studied in various contexts, and there are a few quantum algorithms for controllization proposed under certain assumptions. In this thesis, we seek a general framework for understanding controllization. To this end, we first seek an "appropriate" definition of a controlled version of general quantum operations beyond unitary operations by extending the definition of controlled unitary operations. Our definition is based on two possible physical implementations and one axiomatic approach, and we show that all the three converge to the same definition. We then generalize the definition of controlled quantum operations to a controlled version of higher-order quantum operations. Based on this definition, controllization can be regarded as a controlled version of a certain class of higher-order quantum operations called *neutralization*, and we can analyze the performance of controllization within this definition. We provide a method that reproduces certain previously known quantum algorithms for controllization [17] within this framework. Moreover, we propose a new quantum algorithm for approximate controllization without using auxiliary system, which is not possible in the previously known ones [17, 20].

Success-or-Draw In the last topic, we propose a new structure of higher-order quantum operations named *success-or-draw* for probabilistic higher-order quantum operations, which allows a repeat-until-success implementation of them. Certain higher-order quantum operations such as unitary inversion are known to be implementable in an exact and probabilistic manner. When a probabilistic algorithm is available, a straightforward method for enhancing the success probability is to perform the same algorithm multiple times until success, i.e., a repeat-until-success strategy. Such a strategy requires the input state to be suitably prepared every time when the algorithm is repeated. In order to perform a higher-order quantum operation, the input state on which the output operation is applied is necessary in addition to the input operations. In the classical case, the input state can be copied and re-used multiple times. Thus, it is not a fundamental limitation in the repeat-until-success strategy. In the quantum case, however, the input state cannot be cloned in general [7], and moreover, the input state will be disturbed in general regardless of success or failure. Thus, in order to apply the repeat-until-success strategy for probabilistic higher-order quantum operation, both copies of the input operations and the input state are necessary in general. While the input operation can be "copied" by physically using the corresponding quantum circuit multiple times, the requirement of cloning the input state causes the realization of repeat-until-success strategy difficult practically in the quantum case.

In Ref. [13], an explicit quantum circuit for probabilistic unitary inversion is presented. It utilizes certain properties characteristic to the problem of unitary inversion and shows that it is possible to preserve the input state even when it fails. Thus, it is possible to perform a repeat-until-success strategy, and achieves an exponentially decreasing failure probability for unitary inversion. However, while they show the possibility of preserving the input state on failure on certain problems, it is not known if a similar method can be applied to other problems.

In this thesis, we mathematically identify the structure that guarantees the preservation of the input state on failure as the success-or-draw structure. With the mathematical definition of the success-or-draw structure, we prove that this structure is compatible with a large class of higher-order quantum operations. We also analyze the problem of unitary inversion in terms of success-or-draw, and propose a protocol with a higher success probability than previously known ones.

1.4 Organization of This Thesis

This thesis is organized as follows. In Chapter 2, we review basic mathematical tools used in quantum information and the formulation of higher-order quantum operations. We then review certain higher-order quantum operations related to our main results. In Chapter 3, we analyze the relationship between different definitions of quantum switch and prove that they coincide under two natural assumptions. In Chapter 4, we consider controllization by constructing a theoretical framework of general controlled quantum operations and controlled higher-order quantum operations, and analyze the problem of controllization within this framework. In Chapter 5, we propose a new useful structure of higher-order quantum operations, the success-or-draw structure, and provide a realization theorem of this structure. We also analyze the unitary inversion in terms of the proposed structure. Chapter 6 concludes the thesis and proposes the possible future scope for further study.

Chapter 2

Preliminary

In this chapter, we first introduce the two basic concepts of quantum information theory, quantum states (Sec. 2.1) and quantum operations (Sec. 2.2). We then review the mathematical formalism of higher-order quantum operations in Sec. 2.3 and several results on higher-order quantum operations relevant to the following chapters. In Sec. 2.5, we give a brief introduction to the indefinite causal order and a characteristic higher-order quantum operation for the indefinite causal order known as quantum switch. In Sec. 2.4, we introduce a higher-order quantum operation known as the controllization, which we will focus on in Chapter 4. In Sec. 2.6, we introduce another higher-order quantum operation known as the unitary inversion. The main result of Chapter 5 is inspired by a certain algorithm for unitary inversion, and unitary inversion will also be analyzed in Chapter 5.

2.1 Quantum States

In this thesis, only finite-dimensional systems are considered. A quantum system is described by a Hilbert space as $\mathcal{H} \simeq \mathbb{C}^d$, where d is the dimension of the system. The Hilbert spaces on which the vectors and operators are defined are specified by the subscripts or superscripts, and may be omitted if it is trivial from the context. A two-dimensional quantum system is sometimes called a qubit.

A pure quantum state is described by a unit vector in the Hilbert space as $|\psi\rangle \in \mathcal{H}$. More precisely, a pure quantum state is described by a ray, that is, two quantum states described by the vectors $e^{i\theta}|\psi\rangle$ and $|\psi\rangle$ correspond to the same quantum state because the global phase $e^{i\theta}$ is a non-physical quantity. We define an orthonormal basis $\{|i\rangle\}_{i=0}^{d-1}$ for $\mathcal{H}$ called the computational basis, and an arbitrary pure quantum state can be decomposed in this basis as $|\psi\rangle = \sum_i c_i|i\rangle$ with complex coefficients $\{c_i\}_{i=0}^{d-1}$ satisfying $\sum_i |c_i|^2 = 1$.

Mixed quantum states, which are probabilistic mixtures of pure quantum states, appear in quantum information theory naturally. A mixed state is represented by a linear operator on $\mathcal{H}$ as $\rho \in \mathcal{L}(\mathcal{H})$, which is referred to as a *density operator*. A pure state $|\psi\rangle$ is described by the corresponding projector $|\psi\rangle\langle\psi|$. A mixed state obtained by a probabilistic mixture of quantum states $\{\rho_i\}_i$ according to the probability distribution $\{p_i\}_i$ is given by $\rho = \sum_i p_i\rho_i$. Since a pure state is described by a positive operator $|\psi\rangle\langle\psi| \geq 0$ and a mixed state are a probabilistic mixture of pure states, a general quantum state is described by an operator $\rho \in \mathcal{L}(\mathcal{H})$ satisfying the positivity $\rho \geq 0$ and unit trace $\mathrm{Tr}\rho = 1$.

Quantum coherence is an important measure for quantumness, and is considered to be a key element in quantum computing. For a quantum state, coherence is defined for a fixed basis, usually the computational basis or the eigenbasis of a Hamiltonian of a system, and an intuitive understanding of coherence is that how much a quantum state is in a superposition. A quantum state is not coherent if its density operator is diagonal in that basis, which is a probabilistic mixture of each basis state rather than a superposition. There exist various measures for coherence [42], for example, the norm of the off-diagonal terms of a density operator and the distance from non-coherent states.

Next, we consider composite quantum systems. Given two quantum systems described by the Hilbert spaces $\mathcal{H}_1 \simeq \mathbb{C}^{d_1}$ and $\mathcal{H}_2 \simeq \mathbb{C}^{d_2}$, the composite system is represented by the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$. If the quantum states of the two systems are given by pure states $|\psi_1\rangle$ and $|\psi_2\rangle$ respectively, the quantum state of the composite system is also a pure state and is given by $|\psi_1\rangle \otimes |\psi_2\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$. We sometimes abbreviate this state as $|\psi_1\rangle|\psi_2\rangle$ or $|\psi_1\psi_2\rangle$ for convenience. If a pure state in the composite system can be written as a tensor product of two independent pure states in each system as shown above, it is called a product state. The linearity of quantum mechanics allows the linear combination of quantum states to be a quantum state. If a pure state cannot be decomposed as the tensor product of two pure states in each system, it is called an entangled state. Similarly, if a mixed state can be written as a tensor product as $\rho = \rho_1 \otimes \rho_2 \in \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$, it is called a product state. If a mixed state can be written as a probabilistic mixture of product states as $\rho = \sum_i p_i(\rho_1)_i \otimes (\rho_2)_i$, it is called a separable state, and otherwise an entangled state.

We define a special class of bipartite states, the maximally entangled states. Here we assume that $d_1 = d_2 = d$ for convenience. A bipartite state is said to be a maximally entangled state if it can be written as

$$|\psi\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |e_i^1\rangle |e_i^2\rangle, \tag{2.1}$$

where $\{|e_i^1\rangle\}$ and $\{|e_i^2\rangle\}$ are bases of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. Moreover, such a state can be written as

$$|\psi\rangle = (I \otimes U)|\psi^+\rangle \tag{2.2}$$

with some unitary operator U and the state $|\psi^+\rangle$ defined by

$$|\psi^+\rangle := \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |i\rangle |i\rangle \tag{2.3}$$

using the computational basis $\{|i\rangle\}_{i=0}^{d-1}$. For later convenience, we also define the unnormalized version of maximally entangled states denoted by a dual ket symbol $| \cdot \rangle\rangle$ defined by

$$|U\rangle\rangle := (I \otimes U) \sum_{i=0}^{d-1} |i\rangle |i\rangle, \tag{2.4}$$

where $|I\rangle\rangle = \sqrt{d}|\psi^+\rangle$ holds.

2.2 Quantum Operations and their Representations

In this section, we review quantum operations, which describe transformations between quantum states. We then introduce three commonly used representations of transformations in quantum information: the Kraus representation, the Choi-Jamiołkowski representation, and the Stinespring representation.

Consider a deterministic transformation $\widetilde{\mathcal{A}}$ of a quantum state ρ on $\mathcal{H}$ to a quantum state σ on $\mathcal{K}$.[1] A transformation by a deterministic quantum operation is described by a map $\widetilde{\mathcal{A}}$, which has to preserve the properties of quantum states.

The first condition for a map $\widetilde{\mathcal{A}}$ is the linearity, that is, $\widetilde{\mathcal{A}}$ is a linear map satisfying

$$\widetilde{\mathcal{A}}(p_1\rho_1 + p_2\rho_2) = p_1\widetilde{\mathcal{A}}(\rho_1) + p_2\widetilde{\mathcal{A}}(\rho_2). \tag{2.5}$$

[1] The tilde denotes that it is a transformation between linear operators. This notation will be discussed later when higher-order quantum operations are introduced.

The linearity is required because if an input state ρ of a map $\widetilde{\mathcal{A}}$ is a probabilistic mixture of two states ρ_1 and ρ_2 with probability p_1 and p_2, namely, $\rho = p_1\rho_1 + p_2\rho_2$, then the output state $\widetilde{\mathcal{A}}(\rho)$ should also be the probabilistic mixture of $\widetilde{\mathcal{A}}(\rho_1)$ and $\widetilde{\mathcal{A}}(\rho_2)$, namely, $\widetilde{\mathcal{A}}(\rho) = p_1\widetilde{\mathcal{A}}(\rho_1) + p_2\widetilde{\mathcal{A}}(\rho_2)$. The second condition for a map $\widetilde{\mathcal{A}}$ is the complete positivity, that is, $\widetilde{\mathcal{A}}$ is a *completely positive* (CP) map satisfying

$$(\widetilde{\mathcal{A}} \otimes \widetilde{id}_k)(\rho) \geq 0 \tag{2.6}$$

for all positive operators $\rho \geq 0 \in \mathcal{L}(\mathcal{H}\otimes\mathbb{C}^k)$ with an arbitrary finite-dimensional auxiliary space $\mathbb{C}^k$, where $\widetilde{id}_k$ denotes the identity operation on $\mathbb{C}^k$. The CP condition is required due to the positivity of quantum states, if we apply the transformation $\widetilde{\mathcal{A}}$ on a part of the bipartite system $\mathcal{H} \otimes \mathbb{C}^k$, the resulting state should still be positive. The last condition for a map $\widetilde{\mathcal{A}}$ is the trace-preserving property, that is, $\widetilde{\mathcal{A}}$ is a *trace-preserving* (TP) map satisfying

$$\mathrm{Tr}\,[\widetilde{\mathcal{A}}(\rho)] = \mathrm{Tr}\,\rho, \tag{2.7}$$

for all $\rho \in \mathcal{L}(\mathcal{H})$. The TP condition is required because any operator with unit trace should be transformed into an operator with unit trace and due to the linearity. To summarize, a deterministic quantum operation is described by a CPTP map.

Next, we introduce commonly used representations of quantum operations in quantum information. Note that all of them are representations for linear maps, and the linearity of quantum operations are automatically satisfied.

The first representation we introduce is the *Kraus representation* [41]. In the Kraus representation, a quantum operation $\widetilde{\mathcal{A}}$ transforming a quantum state $\rho \in \mathcal{L}(\mathcal{H})$ into another quantum state $\rho' = \widetilde{\mathcal{A}}(\rho) \in \mathcal{L}(\mathcal{K})$ is represented as

$$\widetilde{\mathcal{A}}(\rho) = \sum_i K_i \rho K_i^\dagger, \tag{2.8}$$

where $\{K_i\}$ is a set of linear operators on $\mathcal{L}(\mathcal{H}, \mathcal{K})$ and is called the *Kraus operators* of the quantum operation $\widetilde{\mathcal{A}}$. The CP condition of quantum operation is automatically satisfied, and the TP condition is given by $\sum_i K_i^\dagger K_i = I$ in the Kraus representation, where I denotes the identity operator on $\mathcal{H}$.

The quantum operation for a unitary operation $\widetilde{\mathcal{U}}$ is represented as $\widetilde{\mathcal{U}}(\rho) = U\rho U^\dagger$ using the corresponding unitary operator U. In this thesis, we also call a unitary operation by the corresponding unitary operator as unitary operation U. The Kraus representation of a unitary operation consists of a single Kraus operator U. Note that the global phases of the Kraus operators do not affect the action of a quantum operation, that is, $\{K_i\}$ and $\{e^{i\theta_i}K_i\}$ lead to the same quantum operation. In general, Kraus operators of a quantum operation are not uniquely determined. Different sets of Kraus operators of a quantum operation exist, and there is a simple relationship between them as follows. Let $\{K_i\}_{i=0}^{n-1}$ and $\{K'_j\}_{j=0}^{n-1}$ represent the same quantum operation, then $K'_j = \sum_i u^*_{ji} K_i$ holds where (u_{ij}) is a unitary matrix. In fact,

$$\sum_j K'_j \rho K'^{\dagger}_j = \sum_{i_1,i_2,j} (u^*_{ji_1} K_{i_1}) \rho (u_{ji_2} K^{\dagger}_{i_2}) = \sum_{i_1,i_2} \delta_{i_1 i_2} K_{i_1} \rho K^{\dagger}_{i_2} = \sum_i K_i \rho K^{\dagger}_i \quad (2.9)$$

holds, and the two sets of Kraus operators represent the same quantum operation.

The second representation the *Choi-Jamiołkowski representation* [43, 44], or simply the Choi representation. In the Choi representation, a quantum operation $\widetilde{\mathcal{A}} : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{K})$ is represented as a linear operator on $\mathcal{H} \otimes \mathcal{K}$ called a Choi operator $J_{\mathcal{A}}$ defined by

$$J_{\mathcal{A}} = (\widetilde{id} \otimes \widetilde{\mathcal{A}})(|I\rangle\rangle\langle\langle I|^{\mathcal{H}\mathcal{H}}) \quad (2.10)$$

where $|I\rangle\rangle := \sum_m |m\rangle|m\rangle$ is the unnormalized maximally entangled state in $\mathcal{H} \otimes \mathcal{H}$ and $\widetilde{id}$ denotes the identity operation on the first system. This relationship between a quantum operation (channel) and a quantum state is known as the Choi-Jamiołkowski isomorphism or the state-channel duality. When a quantum operation $\widetilde{\mathcal{A}}$ is given by Eq. (2.8), the corresponding Choi operator can be written as

$$J_{\mathcal{A}} = \sum_i |K_i\rangle\rangle\langle\langle K_i|^{\mathcal{H}\mathcal{K}}, \quad (2.11)$$

where $|K_i\rangle\rangle \in \mathcal{H} \otimes \mathcal{K}$ is given by

$$|K_i\rangle\rangle = \sum_{mn} \langle m|K_i|n\rangle \cdot |n\rangle|m\rangle. \quad (2.12)$$

In contrast to the the Kraus operators, the Choi operator does not depend on the choice of the Kraus operators and is uniquely determined by $\widetilde{\mathcal{A}}$. Given a Choi operator $J_{\mathcal{A}}$ of a quantum operation $\widetilde{\mathcal{A}}$, the original linear map is obtained by

$$\widetilde{\mathcal{A}}(\rho) = \mathrm{Tr}_{\mathcal{H}}[J_{\mathcal{A}}(\rho^T \otimes I^{\mathcal{K}})] \quad (2.13)$$

for $\rho \in \mathcal{H}$. The CP condition of quantum operation $\widetilde{\mathcal{A}}$ is equivalent to the positivity of the corresponding Choi operator as $J_{\mathcal{A}} \geq 0$, and the TP condition is equivalent to $\mathrm{Tr}_{\mathcal{K}} J_{\mathcal{A}} = I^{\mathcal{H}}$.

For a unitary operation $\widetilde{\mathcal{U}}(\rho) = U\rho U^\dagger$, the corresponding Choi operator is given by

$$J_U = (\widetilde{id} \otimes \widetilde{\mathcal{U}})(|I\rangle\!\rangle\langle\!\langle I|^{\mathcal{H}\mathcal{H}}) \tag{2.14}$$
$$= (I \otimes U)|I\rangle\!\rangle\langle\!\langle I|^{\mathcal{H}\mathcal{H}}(I \otimes U^\dagger) = |U\rangle\!\rangle\langle\!\langle U|^{\mathcal{H}\mathcal{K}}. \tag{2.15}$$

Note that the Choi operator for the identity operation described by the identity operator I on $\mathcal{H}$ to $\mathcal{K}$ is given by $J_{id} = J_I = |I\rangle\!\rangle\langle\!\langle I|$ on $\mathcal{H}\otimes\mathcal{K}$, while the projector appearing $|I\rangle\!\rangle\langle\!\langle I|$ in Eq. (2.10) is an operator on $\mathcal{H} \otimes \mathcal{H}$. Due to the importance of the identity operation in this thesis, we denote the Choi operator for the identity operation as J_{id} instead of J_I.

The last representation is the *Stinespring representation* [45]. Any quantum operation can be realized by a unitary operation on an extended system followed by a projective measurement, and the Stinespring representation is based on this structure. For a quantum operation $\widetilde{\mathcal{A}}$ represented by the Kraus operators $\{K_i\}_{i=0}^{n-1}$, it is always possible to define a unitary operator U on an extended quantum system $\mathcal{H} \otimes \mathcal{H}_{\text{aux}}$ by adding an auxiliary system $\mathcal{H}_{\text{aux}} = \mathbb{C}^n$ satisfying

$$U|\psi\rangle|0\rangle = \sum_{i=0}^{n-1} K_i|\psi\rangle|i\rangle, \tag{2.16}$$

where $\{|i\rangle\}_{i=0}^{n-1}$ is an orthonormal basis of the auxiliary system. We call this U as a purification of the Kraus representation $\{K_i\}$. Similar to the Kraus representation, the Stinespring representation is not unique. The quantum operation $\widetilde{\mathcal{A}}$ can be represented as the reduced dynamics of this unitary operation as

$$\widetilde{\mathcal{A}}(\rho) = \text{Tr}_{\text{aux}}\left[U\left(\rho \otimes |0\rangle\langle 0|\right)U^\dagger\right]. \tag{2.17}$$

Probabilistic Quantum Operations

Probabilistic transformations of quantum states are allowed in quantum mechanics in addition to deterministic ones. Considering that the trace of a density operator corresponds to the probability in the state, and the probability cannot exceed one. The TP condition for deterministic transformation is replaced by the trace-non-increasing (TNI) condition. That is, a probabilistic quantum operation $\widetilde{\mathcal{A}} : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{K})$ transforms a quantum state ρ into $\widetilde{\mathcal{A}}(\rho)$, and the probability of this transformation is given by $\text{Tr}\,\widetilde{\mathcal{A}}(\rho) \leq 1$ in general.

One type of basic probabilistic transformations is a quantum measurement, especially given by the positive operator-valued measurements (POVM). A POVM consists of a set of positive operators $\{\Lambda_i\}_{i=0}^{n-1}$ satisfying $\sum_{i=0}^{n-1} \Lambda_i = I$, and it transforms a quantum state ρ into a probability distribution given by $\{\text{Tr}\,(\Lambda_i\rho)\}_i$.

A general probabilistic quantum operation is described by a set of measurement operators $\{M_i\}_{i=0}^{n-1}$ satisfying $\sum_{i=0}^{n-1} M_i^\dagger M_i = I$, and it transforms a quantum state ρ into a quantum state $M_i \rho M_i^\dagger / \mathrm{Tr}\, M_i^\dagger M_i \rho$ with probability $\mathrm{Tr}\, M_i^\dagger M_i \rho$. It is important that the measurement outcome is known to be i. If the measurement outcome is not given, then the resulting quantum state is given by a probabilistic mixture calculated as $\sum_{i=0}^{n-1} M_i \rho M_i^\dagger$, which is the same state as a deterministic quantum operation given by the Kraus operators $\{M_i\}_{i=0}^{n-1}$. When we say probabilistic quantum operations, we also consider the case that only certain measurement outcomes, say a set given by $\{0, 1, \ldots, m-1\}$ with $m < n$, is obtained by post-selection. In this case, the Kraus operators for this probabilistic quantum operation are given by $\{M_i\}_{i=0}^{m-1}$, and it is easy to see that $\sum_{i=0}^{m-1} M_i^\dagger M_i \leq I$ holds. We say that a probabilistic quantum operation is succeeded if we obtain certain measurement outcomes specified in advance, otherwise failed, and the success part and the failure part sum up to a deterministic quantum operation.

The Choi operator $J_{\mathcal{A}}$ for a probabilistic quantum operation is a positive operator $J_{\mathcal{A}} \geq 0$ satisfying $\mathrm{Tr}_{\mathcal{K}} J_{\mathcal{A}} \leq I^{\mathcal{H}}$. If we call this as success, and assume that $J_F \geq 0$ is a Choi operator corresponds to failure, then it is required that they sum up to a deterministic quantum operation, namely, $J = J_{\mathcal{A}} + J_F$ satisfies $J \geq 0$ and $\mathrm{Tr}_{\mathcal{K}} J = I^{\mathcal{H}}$. Note that J_F is not uniquely determined for a $J_{\mathcal{A}}$ in general.

2.3 Higher-order Quantum Operations

In this section, we introduce *quantum supermaps*, a mathematical tool for describing higher-order quantum operations [11, 12]. Quantum supermaps describes transformations between quantum operations. We first present a formalism for quantum supermaps that are compatible with the quantum circuit model, especially the ones that use the input operations in a fixed order. Such quantum supermaps are called *quantum combs*. We also introduce quantum supermaps with indefinite causal order by relaxing certain requirements for quantum combs. While quantum supermaps with indefinite causal order cannot be implemented within the usual quantum circuit model, there are currently no known physical principles that forbid their implementation, and are expected to provide certain advantages in quantum information processing.

The conditions for quantum supermaps are usually presented in terms of the Choi representation. It is possible to present these conditions in the Kraus representation as we show in Appendix B. In order to avoid confusion, we mainly denote quantum operations with a tilde and supermaps with a double tilde in this thesis. We may omit the tildes when it is not important to distinguish whether a map and a supermap especially when they are referred in the subscript of a Choi operator. For a quantum operation, we denote a map by $\widetilde{\mathcal{A}} : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{K})$ and its Choi operator by $J_{\mathcal{A}} \in \mathcal{L}(\mathcal{H} \otimes \mathcal{K})$. For a higher-order quantum operation transforming a quantum operation $\widetilde{\mathcal{A}} : \mathcal{L}(\mathcal{I}_1) \to \mathcal{L}(\mathcal{O}_1)$ to a quantum operation $\widetilde{\mathcal{A}}' : \mathcal{L}(\mathcal{I}_0) \to \mathcal{L}(\mathcal{O}_0)$, we denote the supermap as $\widetilde{\widetilde{\mathcal{S}}} : [\mathcal{L}(\mathcal{I}_1) \to \mathcal{L}(\mathcal{O}_1)] \to [\mathcal{L}(\mathcal{I}_0) \to \mathcal{L}(\mathcal{O}_0)]$. It is possible to describe the supermap as a map transforming the Choi operators of the input and the output quantum operations, which we describe as $\widetilde{\mathcal{S}} : \mathcal{L}(\mathcal{I}_1 \otimes \mathcal{O}_1) \to \mathcal{L}(\mathcal{I}_0 \otimes \mathcal{O}_0)$. The Choi operator for this supermap is given by an operator $S \in \mathcal{L}(\mathcal{I}_1 \otimes \mathcal{O}_1 \otimes \mathcal{I}_0 \otimes \mathcal{O}_0)$. Note that the order of the Hilbert spaces may vary for convenience, and we denote the order of the Hilbert spaces explicitly when it is ambiguous. The conditions for the supermaps in terms of the corresponding Choi operators are given in the following.

2.3.1 Quantum Combs

The most general way to transform a set of input operations $\widetilde{\Lambda}_1, \ldots, \widetilde{\Lambda}_K$ is to insert quantum operations before and after each input operation as the quantum circuit shown in Fig. 2.1, if the usage of the input operations is fixed and given by this order. Let the input and the output Hilbert spaces for input operations $\widetilde{\Lambda}_k$ be $\mathcal{I}_k$ and $\mathcal{O}_k$, the corresponding Choi operators be L_k, the auxiliary systems be $\mathcal{A}_k$, and the input and the output Hilbert spaces for the output operation be $\mathcal{I}_0$ and $\mathcal{O}_0$, respectively, as shown in the quantum circuit in Fig. 2.1 for $K = 2$. Let the quantum operations inserted be $\widetilde{\mathcal{E}}_1 : \mathcal{L}(\mathcal{I}_0) \to \mathcal{L}(\mathcal{I}_1 \otimes \mathcal{A}_1), \widetilde{\mathcal{E}}_2 : \mathcal{L}(\mathcal{O}_1 \otimes \mathcal{A}_1) \to \mathcal{L}(\mathcal{I}_2 \otimes \mathcal{A}_2), \ldots, \widetilde{\mathcal{E}}_K : \mathcal{L}(\mathcal{O}_{K-1} \otimes \mathcal{A}_{K-1}) \to \mathcal{L}(\mathcal{I}_K \otimes \mathcal{A}_K), \widetilde{\mathcal{E}}_{K+1} : \mathcal{L}(\mathcal{I}_K \otimes \mathcal{A}_K) \to \mathcal{L}(\mathcal{O}_0)$, and the corresponding Choi operators be $E_1, E_2, \ldots, E_K, E_{K+1}$. Then a quantum comb $\widetilde{\widetilde{\mathcal{C}}}$ transforms the input operations $\widetilde{\Lambda}_1, \ldots, \widetilde{\Lambda}_K$ as

$$\widetilde{\widetilde{\mathcal{C}}}(\widetilde{\Lambda}_1, \ldots, \widetilde{\Lambda}_K) = \widetilde{\mathcal{E}}_{K+1} \circ (\widetilde{\Lambda}_K \otimes \widetilde{id}_{\mathcal{A}_K}) \circ \widetilde{\mathcal{E}}_K \circ \cdots \circ \widetilde{\mathcal{E}}_2 \circ (\widetilde{\Lambda}_1 \otimes \widetilde{id}_{\mathcal{A}_1}) \circ \widetilde{\mathcal{E}}_1. \quad (2.18)$$

In the Choi representation, the l.h.s should be equal to

$$\mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1\cdots\mathcal{I}_K\mathcal{O}_K}[C(L_1 \otimes \cdots \otimes L_K)^T], \quad (2.19)$$

where C is the Choi operator of the quantum comb $\widetilde{\widetilde{\mathcal{C}}}$. The r.h.s. is given by

$$\begin{aligned} &\mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1\mathcal{A}_1\cdots\mathcal{I}_K\mathcal{O}_K\mathcal{A}_K}(E_{K+1}L_K^T E_K^{T_{\mathcal{A}_K}} \cdots E_2^{T_{\mathcal{A}_2}} L_1^T E_1^{T_{\mathcal{A}_1}}) && (2.20)\\ &= \mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1\mathcal{A}_1\cdots\mathcal{I}_K\mathcal{O}_K\mathcal{A}_K}[(E_{K+1}E_K^{T_{\mathcal{A}_K}} \cdots E_2^{T_{\mathcal{A}_2}} E_1^{T_{\mathcal{A}_1}})(L_1 \otimes \cdots \otimes L_K)^T], && (2.21)\end{aligned}$$

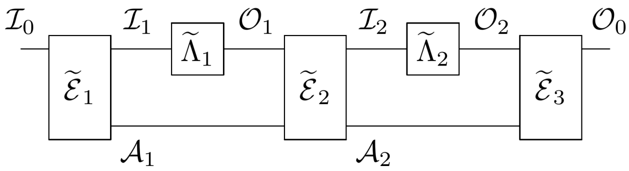


Figure 2.1: The most general way for implementing a quantum comb (a quantum supermap with definite order of input operations) with two input operations $\widetilde{\Lambda}_1$ and $\widetilde{\Lambda}_2$ in the quantum circuit model.

where $T_{\mathcal{A}_K}$ denotes the partial transpose on $\mathcal{A}_K$, and the equality holds because L_k are the operators on different Hilbert spaces for different k and the partial trace is taken on $\mathcal{I}_k$ and $\mathcal{O}_k$ for all $k \geq 1$. Note that the identity operators are omitted. Thus, the Choi operator of the quantum comb C is given by concatenating the quantum operations $E_1, \dots, E_{K+1}$ and tracing out the auxiliary systems $\mathcal{A}_1, \dots, \mathcal{A}_K$ as

$$C = \mathrm{Tr}_{\mathcal{A}_1 \cdots \mathcal{A}_K}(E_{K+1} E_K^{T_{\mathcal{A}_K}} \cdots E_2^{T_{\mathcal{A}_2}} E_1^{T_{\mathcal{A}_1}}). \tag{2.22}$$

In the following, we present the condition for C by considering the conditions for $E_1, \dots, E_{K+1}$.

The first condition for the Choi operator of a quantum comb C is that it is a positive operator $C \geq 0$. This is because every quantum operation $\widetilde{\mathcal{E}}_k$ is CP, the concatenation of them is also CP, thus the corresponding Choi operator C is positive. The second condition for C is given by a set of linear constraints

$$\mathrm{Tr}_{\mathcal{O}_0} C = C^{(K)} \otimes \frac{I^{\mathcal{O}_K}}{d}, \tag{2.23}$$

$$\mathrm{Tr}_{\mathcal{I}_k} C^{(k)} = C^{(k-1)} \otimes \frac{I^{\mathcal{O}_{k-1}}}{d} \quad (2 \leq k \leq K), \tag{2.24}$$

$$\mathrm{Tr}_{\mathcal{I}_1} C^{(1)} = (\mathrm{Tr} C) \frac{I^{\mathcal{I}_0}}{d_0}, \tag{2.25}$$

where $C^{(K)} = \mathrm{Tr}_{\mathcal{O}_K \mathcal{O}_0} C$ and $C^{(k-1)} = \mathrm{Tr}_{\mathcal{O}_{k-1} \mathcal{I}_k} C^{(k)}$ for $k = 2, \dots, K$. These conditions are obtained by the TP condition of each quantum operation E_k. These conditions also indicate that the output state of the quantum comb on $\mathcal{I}_k$ does not depend on the input state of the quantum comb $\mathcal{O}_{k'}$ for $k' \geq k$, that are the input states appear at later times. For that reason, these conditions are known as the *causal condition* for quantum comb. The normalization condition is given by $\mathrm{Tr}\, C = d_{\mathcal{I}_0} d_{\mathcal{O}_1} \cdots d_{\mathcal{O}_K}$. For example, $C = I^{\mathcal{I}_0} \otimes \frac{I^{\mathcal{I}_1}}{d_{\mathcal{I}_1}} \otimes I^{\mathcal{O}_1} \otimes \cdots \otimes I^{\mathcal{O}_K} \otimes \frac{I^{\mathcal{O}_0}}{d_{\mathcal{O}_0}}$ is a deterministic comb. It is also shown that the inverse holds [11, 12], that is, every operator C satisfying the positivity $C \geq 0$ and the causal condition Eq. (2.23)-(2.25) can be implemented by a quantum circuit shown in Fig. 2.1.

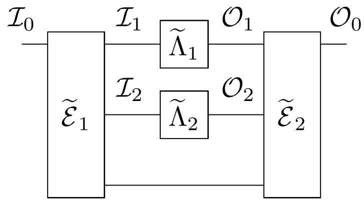


Figure 2.2: A limited class of quantum combs that utilize all input operations, $\widetilde{\Lambda}_1$ and $\widetilde{\Lambda}_2$, in a parallel way.

The causal condition given by Eq. (2.23)-(2.25) is also known as the *sequential condition*, because it assumes sequential uses of the input operations. It is also possible to consider the case where all input operations are used in a parallel way as shown in the quantum circuit in Fig. 2.2. In this case, it is equivalent to the 1-slot quantum comb, where the input and output Hilbert spaces of the slot are given by $\mathcal{I} := \mathcal{I}_1 \otimes \cdots \otimes \mathcal{I}_K$ and $\mathcal{O} := \mathcal{O}_1 \otimes \cdots \otimes \mathcal{O}_K$. That is, the parallel condition is given by

$$\mathrm{Tr}_{\mathcal{O}_0} C = \mathrm{Tr}_{\mathcal{O}\mathcal{O}_0} C \otimes \frac{I^{\mathcal{O}}}{d_{\mathcal{O}}}. \tag{2.26}$$

$$\mathrm{Tr}_{\mathcal{I}\mathcal{O}\mathcal{O}_0} C = (\mathrm{Tr} C) \frac{I^{\mathcal{I}}}{d_{\mathcal{I}}}. \tag{2.27}$$

In the formulation of the quantum comb, the dimensions of the auxiliary systems are not restricted except that they are finite. Thus, any quantum comb with the parallel condition is simply a restricted version of a general quantum comb, i.e., a quantum comb with the sequential condition. While the quantum comb with the sequential condition is more general, the parallel condition has been relatively well-studied for various reasons. The parallel condition treats all the input operations in the same way, thus there is a higher symmetry between the input operations. A quantum comb with the parallel condition also has an advantage in that it can be performed in a shorter time compared to the sequential case. Moreover, there are various physical systems that can apply the same quantum operations to multiple quantum states, in which case the parallel condition is achieved naturally. Note that it is also possible to consider certain causal conditions partially parallel or partially sequential.

Probabilistic Quantum Combs

Next, we introduce the *probabilistic quantum combs*. Similar to the probabilistic quantum operations, probabilistic quantum combs are obtained by inserting probabilistic quantum operations before and after each input operation. A probabilistic quantum comb is implementable if there exists another probabilistic quantum comb such that they sum up to a deterministic quantum comb. In the Choi representation, a probabilistic quantum operation is described by a positive operator J_Λ satisfying $J_\Lambda \leq J$ where J is the Choi operator of a deterministic quantum operation. Similarly, a probabilistic quantum comb is described by a positive operator $S \geq 0$ satisfying $S \leq C$ where C is the Choi operator of a deterministic quantum comb. We usually consider a probabilistic higher-order quantum operation with two labels, success and failure, which are represented by S and F. In this case, the conditions for S and F are given by

$$S \geq 0, \quad F \geq 0 \tag{2.28}$$

$$S + F \text{ is a deterministic comb.} \tag{2.29}$$

2.3.2 Higher-order Quantum Operations with Indefinite Causal Order

The requirements for a quantum comb basically originate from the requirements that it transforms input quantum operations into an output quantum operation, and there is a causal order between the usage of each input operation. However, the second condition is a requirement that comes from the fact that we use the input operations in a fixed order, and it is not a fundamental restriction for higher-order quantum operations. Instead of requiring the causal condition of the quantum comb, or the sequential condition, we can consider a relaxed version: a quantum supermap transforming CPTP maps into CPTP maps.

A simple example that satisfies this assumption is a probabilistic mixture of different orders of the usage of the input operations. For simplicity, we consider the case $K = 2$, where there exist only two input operations $\widetilde{\Lambda}_1$ and $\widetilde{\Lambda}_2$. In this case, it is possible to probabilistically choose to use $\widetilde{\Lambda}_1$ or $\widetilde{\Lambda}_2$ first and the other for the second. We then obtain a quantum operation given by $\frac{1}{2}(\widetilde{\Lambda}_1 \circ \widetilde{\Lambda}_2 + \widetilde{\Lambda}_2 \circ \widetilde{\Lambda}_1)$. This is a valid higher-order quantum operation and it does not satisfy the causal condition Eq. (2.23)-(2.25). A more non-trivial example is quantum switch [27] which will be introduced in Sec. 2.5.

The condition for indefinite causal order in terms of the Choi representation is not simple in general. Here we only present the case of $K = 2$ [29]. A supermap W is a valid supermap within indefinite causal order if it satisfies

$$W \geq 0 \tag{2.30}$$
$$\mathrm{Tr}_{\mathcal{O}_0} W = \mathrm{Tr}_{\mathcal{O}_1 \mathcal{O}_0} W + \mathrm{Tr}_{\mathcal{O}_2 \mathcal{O}_0} - \mathrm{Tr}_{\mathcal{O}_1 \mathcal{O}_2 \mathcal{O}_0} \tag{2.31}$$
$$\mathrm{Tr}_{\mathcal{I}_2 \mathcal{O}_2 \mathcal{O}_0} W = \mathrm{Tr}_{\mathcal{O}_1 \mathcal{I}_2 \mathcal{O}_2 \mathcal{O}_0} W \tag{2.32}$$
$$\mathrm{Tr}_{\mathcal{I}_1 \mathcal{O}_1 \mathcal{O}_0} W = \mathrm{Tr}_{\mathcal{O}_2 \mathcal{I}_1 \mathcal{O}_1 \mathcal{O}_0} W \tag{2.33}$$
$$\mathrm{Tr}_{\mathcal{I}_1 \mathcal{O}_1 \mathcal{I}_2 \mathcal{O}_2 \mathcal{O}_0} W = \mathrm{Tr} W. \tag{2.34}$$

The condition for $K = 3$ is presented in Ref. [14]. While these conditions are more complex than the sequential condition, it is invariant under the permutation of input operations. Thus, even if what we focus on is the sequential condition, it is sometimes useful to consider the indefinite causal order, which may simplify the problem by investigating certain symmetries.

2.3.3 Higher-order Quantum Operations with Multiple Copies of an Input Operation

We have stated the conditions for a higher-order quantum operation to be implementable, in the sense that whether the transformation from a set of input operations $\widetilde{\Lambda}_1, \ldots, \widetilde{\Lambda}_K$ to the target output operation is possible. Here only a single use of each input operation is allowed, but multiple uses of each input operation can be considered in general.

For simplicity, we consider the transformation of an input operation $\widetilde{\Lambda}_I$ to an output operation $\widetilde{\Lambda}_O$. If we are allowed to use K copies of $\widetilde{\Lambda}_I$ and implement $\widetilde{\Lambda}_O$, the corresponding quantum supermap satisfies $\widetilde{\widetilde{\mathcal{S}}} : \widetilde{\Lambda}_I^{\otimes K} \mapsto \widetilde{\Lambda}_O$. That is, the action of $\widetilde{\widetilde{\mathcal{S}}}$ on multiple copies of an input operation $\widetilde{\Lambda}_I^{\otimes K}$ is defined, but its action on other input operations such as $\widetilde{\Lambda}_1 \otimes \widetilde{\Lambda}_2 \otimes \cdots \otimes \widetilde{\Lambda}_K$ with all different $\widetilde{\Lambda}_i$ is not necessarily defined. The positivity and the causal conditions for the supermap S are still required for implementing this supermap. However, there is more freedom in defining the action of the supermap, and thus a larger class of higher-order quantum operations is implementable under the multiple copy scenario.

2.4 Controlled Unitary Operations and Controllization

In this section, we review the higher-order quantum operation known as controllization [19–25], a higher-order quantum operation transforming unitary operation into its controlled version. Controllization can be considered to be a quantum counterpart of the “if clause” in classical computing. It is shown that controllization is not possible under certain assumptions. By relaxing some of the assumptions, there are a few quantum algorithms for implementing controllization. In this section, we review the preceding results on the problem of controllization.

2.4.1 Controlled Unitary Operations

We first review some properties of controlled unitary operations. Controlled unitary operations are a special class of unitary operations which can be regarded as conditional operations. In classical computation, a conditional operation is defined for two systems, a control system and a target system. The action of a conditional operation is to apply an operation if the control bit is in state 1, and do nothing if the control bit is in state 0. A controlled unitary operation is a quantum counterpart of such a conditional operation, acting on a control quantum system and a target quantum system. Conventionally, a controlled unitary operation is a unitary operation that applies the target unitary operation or the identity operation on the target system *coherently* depending on the state of the control qubit. For a d-dimensional unitary operation represented by a unitary operator $U : \mathcal{H}(:= \mathbb{C}^d) \to \mathcal{K}(:= \mathbb{C}^d)$, the corresponding controlled unitary operation $\widetilde{\mathcal{C}}_U$ is defined by a unitary operator $C_U : \mathcal{H}_C \otimes \mathcal{H} \to \mathcal{K}_C \otimes \mathcal{K}$ with the control systems $\mathcal{H}_C = \mathbb{C}^2$ and $\mathcal{K}_C = \mathbb{C}^2$ given by

$$C_U := |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes e^{i\theta_U} U, \tag{2.35}$$

where θ_U is an arbitrary phase factor. The corresponding Choi operator $J_{\mathcal{C}_U} \in \mathcal{L}(\mathcal{H}_C \otimes \mathcal{K}_C \otimes \mathcal{H} \otimes \mathcal{K})$ is given by

$$\begin{aligned} J_{\mathcal{C}_U} &= (|00\rangle|I\rangle\rangle + |11\rangle|e^{i\theta_U}U\rangle\rangle)(\langle 00|\langle\langle I| + \langle 11|\langle\langle e^{i\theta_U}U|) & (2.36)\\ &= |00\rangle\langle 00| \otimes J_{id} + |11\rangle\langle 11| \otimes J_U \\ &\quad + |00\rangle\langle 11| \otimes |I\rangle\rangle\langle\langle e^{i\theta_U}U| + |11\rangle\langle 00| \otimes |e^{i\theta_U}U\rangle\rangle\langle\langle I| & (2.37) \end{aligned}$$

where $|ii\rangle \in \mathcal{H}_C \otimes \mathcal{K}_C$ for $i, j = 0, 1$ is the state of the control qubit system. The degree of freedom of the phase factor θ_U is required in the definition, because while unitary operators U and $e^{i\phi}U$ with a global phase $\phi \in \mathbb{R}$ representing the same unitary operation $\widetilde{\mathcal{U}}$, the corresponding controlled unitary operations $|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U$ and $|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes e^{i\phi}U$ corresponds to different unitary operations. This phase factor cannot be determined just by specifying the unitary operation $\widetilde{\mathcal{U}}$, even if we restrict U to be an element of $\mathrm{SU}(d)$, in which case the degree of freedom of the phase factor $e^{\frac{2\pi i}{d}}$ still remains.

An important characteristic of the controlled unitary operation $\widetilde{\mathcal{C}}_U$ defined by Eq. (2.35) is that it preserves coherence between the output states with the control system being in $|0\rangle$ and $|1\rangle$. This coherence can be evaluated by a norm of the off-diagonal term of its Choi operator, namely, the terms with the control systems $|00\rangle\langle 11|$ and $|11\rangle\langle 00|$ in Eq. (2.37). An incoherent version of a controlled unitary operation can also be defined by the Choi operator given by

$$J_{\mathcal{C}_U^{\mathrm{cls}}} = |00\rangle\langle 00| \otimes J_{id} + |11\rangle\langle 11| \otimes J_U, \tag{2.38}$$

and we call $J_{\mathcal{C}_U^{\mathrm{cls}}}$ as a classically controlled version of a unitary operation represented by U. Such a classically controlled operation can be implemented by first measuring the control qubit on the computational basis, and then applying the unitary operation or the identity operation depending on the measurement outcome. Note that while a generalization of coherently controlled unitary operation is not straightforward, this classically controlled unitary operation can be easily generalized to the classically controlled version of general quantum operation $\widetilde{\mathcal{A}}$ as

$$J_{\mathcal{C}_{\mathcal{A}}^{\mathrm{cls}}} := |00\rangle\langle 00| \otimes J_{id} + |11\rangle\langle 11| \otimes J_{\mathcal{A}}. \tag{2.39}$$

2.4.2 Controllization and No-go Theorem

Controllization is a higher-order quantum operation transforming a unitary operation into a corresponding controlled unitary operation. A straightforward definition of controllization is given by a map on corresponding unitary operators as $U \mapsto |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U$. However, this map does not define a supermap, because a unitary operation $\widetilde{\mathcal{U}}$ can be described by any unitary operator of the form $e^{i\theta}U$ with the global phase $e^{i\theta}$. To avoid inconsistency about the global phase, a phase factor is usually introduced to cancel out the effect of the global phase in the definition of controllization. That is, we define controllization by a map $U \mapsto |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes e^{i\theta_U}U$, where θ_U is an arbitrary phase factor depending on U. By introducing this phase factor θ_U, a supermap from a unitary operation $\widetilde{\mathcal{U}}$ to a corresponding controlled unitary operation can be defined as

$$\widetilde{\mathcal{U}} \mapsto \widetilde{\mathcal{C}}_U, \tag{2.40}$$

where $\widetilde{\mathcal{C}}_U$ denotes the unitary operation defined by the unitary operator given by Eq. (2.35). Note that the phase factor θ_U is included in the definition Eq. (2.35).

The supermap given by Eq. (2.40) is a well-defined supermap, especially an injection, due to the existence of the phase factor. However, it is not trivial if this supermap can be linear for some phase factor, and its implementability in quantum mechanics is not obvious. In Refs. [21–24], it has been shown that this supermap cannot be linear for any phase factor, and thus controllization is not implementable with a single use of the input unitary operation. In Ref. [25], controllization for a restricted set of unitary operations is investigated, and a necessary and sufficient condition for the set of unitary operations is derived.

2.4.3 Possible Workarounds for Controllization

While exact controllization is not possible with a single use of the input unitary operation, there are many attempts to implement controllization with certain relaxations. Here we present two possible workarounds.

Approximate Controllization

The first attempt to implement controlled unitary operation is to implement it in an approximate manner. In Refs. [16, 17], the optimal average fidelity for controllization has been analyzed. Here the average fidelity defined as

$$F := \frac{1}{(2d)^2} \int dU F(J_{\mathcal{C}_U^0}, \widetilde{\mathcal{C}}(J_U)) \tag{2.41}$$

is considered, where $\widetilde{\mathcal{C}}$ denotes a (corresponding map of a) supermap and $\mathcal{C}_U^0 := |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U$ is a controlled unitary operation with a fixed phase factor. The fidelity between the two Choi operators A, B is given by $F(A, B) := \mathrm{Tr}[AB]$. In Ref. [16], the optimal fidelity with a single use of an input operation is obtained as

$$\max_{\widetilde{\mathcal{C}}} F = 1/2 \tag{2.42}$$

by optimizing over all possible deterministic supermap $\widetilde{\mathcal{C}}$. In Ref. [17], the optimal fidelity with multiple uses of an input operation is also obtained by investigating the effect of fixed phase factor in the definition of fidelity, and is shown to be 1/2, the same value as the single use case. This average fidelity is actually achievable in a classical manner, that is, the supermap $\widetilde{\mathcal{U}} \mapsto \widetilde{\mathcal{C}}_U^{\mathrm{cls}}$ achieves this fidelity, where $\widetilde{\mathcal{C}}_U^{\mathrm{cls}}$ is defined by Eq. (2.38).

Controllization for Hamiltonian Dynamics

The second attempt to implement controllization is to consider the case when the unitary operation is given by Hamiltonian dynamics. If a unitary operation is generated by time-independent Hamiltonian dynamics as $U = e^{iHt}$ where we

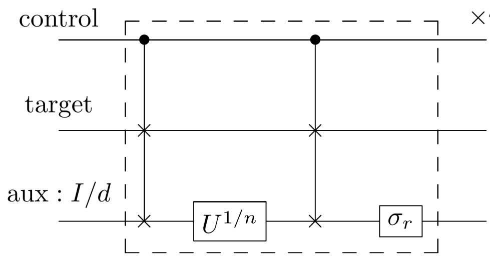


Figure 2.3: The quantum circuit for approximate controllization proposed in Ref. [20]. The initial state of the auxiliary system is given by the completely mixed state I/d. In each iteration, a controlled swap operation, $U^{1/n}$, controlled swap operation, and a random Pauli operation denoted by σ_r are applied in order.

set $\hbar = 1$, we assume that it is possible to divide the time interval t to t/n for some n, so that we can utilize $U^{1/n} = e^{iHt/n}$ instead of U itself.

In Ref. [20], an algorithm implementing approximate controllization with n uses of $U^{1/n}$ is presented. The algorithm is described by the quantum circuit shown in Fig. 2.3. The key element of this algorithm is to keep the auxiliary system in the completely mixed state by randomization with the random Pauli operations $\{\sigma_r\}_r$ after each iteration. The error of this algorithm is measured by the diamond norm [3], which characterizes a distance between two general quantum operations, between the obtained quantum operation and the target controlled unitary operation, and is obtained as $O(1/n)$. In the limit of large n, this algorithm converges to exact controllization.

In Ref. [17], an algorithm implementing exact controllization with d uses of $U^{1/d}$ is presented, where d is the dimension of the unitary operation U. The algorithm is described by the quantum circuit shown in Fig. 2.4. The key element of this algorithm is the totally antisymmetric state

$$|A_d\rangle := \frac{1}{\sqrt{d!}} \sum_{\sigma \in \mathcal{S}_d} \mathrm{sgn}(\sigma) |\sigma(1)\rangle |\sigma(2)\rangle \cdots |\sigma(d)\rangle, \tag{2.43}$$

which is an invariant state under $U^{\otimes d}$ as $U^{\otimes d}|A_d\rangle = det(U)|A_d\rangle$ for an arbitrary unitary operator U. This algorithm achieves exact controllization with a finite division of the original unitary operation.

While the two algorithms both implement controllization, their mathematical characterization is not trivial from the presented algorithms. In Chap. 4, we present a framework for controlled quantum operations, and a unified way for

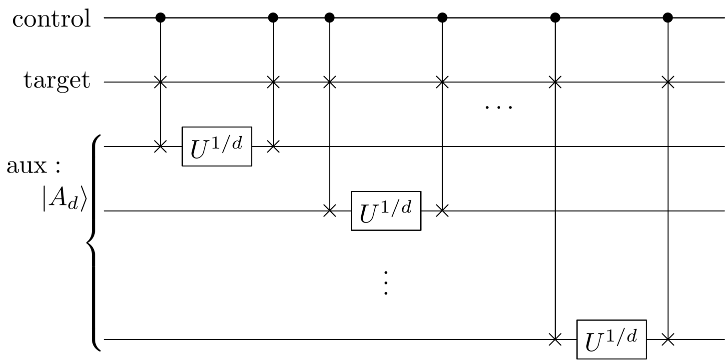


Figure 2.4: The quantum circuit for exact controllization proposed in Ref. [17]. The initial state of the auxiliary system is given by the totally antisymmetric state $|A_d\rangle$.

understanding these algorithms as a result.

2.5 Quantum Switch

Quantum switch [27] is a higher-order quantum operation that transforms multiple input operations into a "coherent superposition of different orders" of the input operations. It is an example of a higher-order quantum operation that cannot be implemented within quantum circuit model, but there is no fundamental principle that forbids its implementation in quantum mechanics. For that, quantum switch is a well-studied higher-order quantum operation in the context of indefinite causal order, for revealing how the causal structure may affect the quantum information processing in quantum mechanics. It is also proposed as a resource for quantum information processing, as it has been shown to provide computational advantage on certain tasks such as discriminating quantum channels [31,32,46] and enhancing communications [33–36,47,48]. Here we only consider quantum switch that uses only two input operations introduced in Ref. [27]. The action of quantum switch can be generalized to multiple input operations as studied in Ref. [32],

2.5.1 Definition of Quantum Switch

The action of quantum switch is to produce a coherent control of causal orders. In Ref. [27], the action of quantum switch is originally defined on unitary operations, and then generalized to quantum operations beyond unitary operations as follows.

Given two unitary operations U_1 and U_2 as input operations, a quantum switch transforms them into the coherent control of different orders, namely, the unitary operation given by

$$W = |0\rangle\langle 0| \otimes U_2 U_1 + |1\rangle\langle 1| \otimes U_1 U_2, \tag{2.44}$$

by using each of U_1 and U_2 only once. If the control qubit is in $|0\rangle$, U_1 is applied on the target system first, and followed by U_2, and if the control qubit is in $|1\rangle$, U_2 is applied first followed by U_1. If the control qubit is in a superposition of $|0\rangle$ and $|1\rangle$, then the two different orders should be "superposed" in a coherent way.

The action of quantum switch for unitary operations is defined in a natural way, and it can be generalized to quantum operations other than unitary operations [27]. Given two quantum operations $\widetilde{\mathcal{A}}_1$ and $\widetilde{\mathcal{A}}_2$ with the Kraus operators $\{K_i\}_i$ and $\{L_j\}_j$ as input operations, a quantum switch transforms them into the quantum operation given by the Kraus operators $\{W_{ij}\}_{ij}$ with

$$W_{ij} = |0\rangle\langle 0| \otimes L_j K_i + |1\rangle\langle 1| \otimes K_i L_j. \tag{2.45}$$

It is easy to see that if two quantum operations are unitary operations, it coincides with the definition for unitary operation. While the Kraus representation is not unique and different Kraus operators can be used for representing the same quantum operation, this definition does not depend on the choice of Kraus operators, which can be checked by using the relationship between different Kraus operators presented in Sec. 2.2.

2.5.2 Superactivation with Quantum Switch

While the action of quantum switch on unitary operations is to simply produce a coherent control of different order, its action on general quantum operations is not necessarily the same.

A simple example is the case where two input operations are identical. If the two input operations are the same unitary operation U, then the output is the unitary operation $|0\rangle\langle 0| \otimes U^2 + |1\rangle\langle 1| \otimes U^2 = I \otimes U^2$, or equivalently, $\widetilde{id} \otimes \widetilde{\mathcal{U}} \circ \widetilde{\mathcal{U}}$. However, if the two input operations are the depolarizing channel $\widetilde{\mathcal{D}}$, the output operation is different from $\widetilde{id} \otimes \widetilde{\mathcal{D}} \circ \widetilde{\mathcal{D}} = \widetilde{id} \otimes \widetilde{\mathcal{D}}$ as follows [33]. For d-dimensional system, the Kraus operators for the depolarizing channel can be chosen as $\{\frac{1}{d} U_i\}_{i=0}^{d^2-1}$ where $\{U_i\}_{i=0}^{d^2-1}$ is a set of unitary operators satisfying $\operatorname{Tr} U_i U_j^\dagger = d\delta_{ij}$. Assuming the control qubit is in $\sqrt{p}|0\rangle + \sqrt{1-p}|1\rangle$, and the target system is given by ρ, the action of the output operation of quantum switch on this input state is given by

$$(p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1|) \otimes \frac{I}{d} + \sqrt{p(1-p)}(|0\rangle\langle 1| + |1\rangle\langle 0|) \otimes \frac{\rho}{d^2}. \tag{2.46}$$

If the control qubit is in $|0\rangle$ or $|1\rangle$, equivalently $p = 1$ or $p = 0$, the target system is given by the completely mixed state I/d, which is expected as the depolarizing channel transforms any input state into the completely mixed state I/d. This also coincides with the case if the output operation is given by $\widetilde{id} \otimes \widetilde{\mathcal{D}}$. However, if the control qubit is in a superposition of $|0\rangle$ and $|1\rangle$, the target system does depend on the input state as Eq. (2.46) shows, and thus the action is different from $\widetilde{id} \otimes \widetilde{\mathcal{D}}$.

This result is surprising because the depolarizing channel does not transfer any information, but when we apply the depolarizing channel twice with the assist of quantum switch, the output operation is not a depolarizing channel anymore, and can be used for transferring information. This phenomenon that quantum switch enables some communication with the depolarizing channel has been studied theoretically in Ref. [33–35], and also experimentally in Ref. [47,48]. As this phenomenon was first pointed out for quantum switch, some consider that such enhancement in communication originates from the indefinite causal order aspect of quantum switch. However, it is also pointed out that such a phenomenon can happen in systems exploiting coherently controlled quantum operations without causally indefinite elements [49, 50].

2.6 Unitary Inversion

In this section, we review the higher-order quantum operation known as unitary inversion [13–17, 38, 39], a higher-order quantum operation transforming unitary operation U into its inverse U^{-1}. Since the inverse of a unitary operation U is given by its Hermitian conjugate, the problem of unitary inversion can be further divided into two higher-order quantum operations: the unitary conjugation, transforming a unitary operation U into its complex conjugate U^*, and the unitary transposition, transforming a unitary operation U into its transposition U^T. Note that while unitary inversion is basis independent, both unitary conjugation and unitary transposition are basis dependent, and both complex conjugate and transposition are defined with respect to the computational basis $\{|i\rangle\}_{i=0}^{d-1}$.

The problem of unitary inversion has been studied in various conditions, for example, approximate cases or probabilistic but exact cases. Since probabilistic but exact supermaps can always be transformed into a deterministic but approximate one by considering the probabilistic mixture of success and failure cases, we do not focus on this difference in this section. Another important feature is how the input unitary operations are used, especially, three types are usually considered: parallel, sequential, and indefinite causal order.

In Ref. [51], a deterministic and exact algorithm for unitary conjugation is presented. The complex conjugate of a unitary operation U can be obtained by using $d-1$ copies of the input unitary operation in a parallel way. Especially, the following equality holds

$$U^* = V^\dagger U^{\otimes d-1} V, \tag{2.47}$$

where V is an isometry defined as

$$V = \frac{1}{\sqrt{(d-1)!}} \sum_{\sigma \in \mathcal{S}_d} \mathrm{sgn}(\sigma) |\sigma(1)\rangle |\sigma(2)\rangle \cdots |\sigma(d-1)\rangle \langle \sigma(d)|, \tag{2.48}$$

with the d-dimensional symmetric group $\mathcal{S}_d$ and permutation σ. Moreover, it is also shown in Ref. [13,14] that unitary conjugation is not possible with less than $d-1$ uses of the input unitary operation even in a probabilistic way. With these results on unitary conjugation, the remaining difficulty for unitary inversion is similar to the difficulty of unitary transposition. In the following of this section, we review the unitary inversion and unitary transposition.

2.6.1 Parallel Strategy

We first review the unitary inversion and unitary transposition with parallel uses of input operations [13, 14, 39]. Let K be the number of uses of the input operation U. The optimal success probability for unitary transposition can be obtained by the following optimization problem

$$\max p \tag{2.49}$$

$$\text{s.t.} \quad \mathrm{Tr}_{\mathcal{IO}}[S J_U^{\otimes K}] = p J_{U^T} \tag{2.50}$$

$$0 \leq S \leq C \tag{2.51}$$

$$C \text{ is a parallel deterministic comb,} \tag{2.52}$$

where S and C are the Choi operator of supermaps. The first constraint defines the action of S to be unitary transposition, and the remaining constraints are the conditions that S is compatible with the quantum circuit model. This optimization problem is also known as semidefinite programming (SDP). In Ref. [14], the optimal success probability for unitary transposition is obtained as a solution to

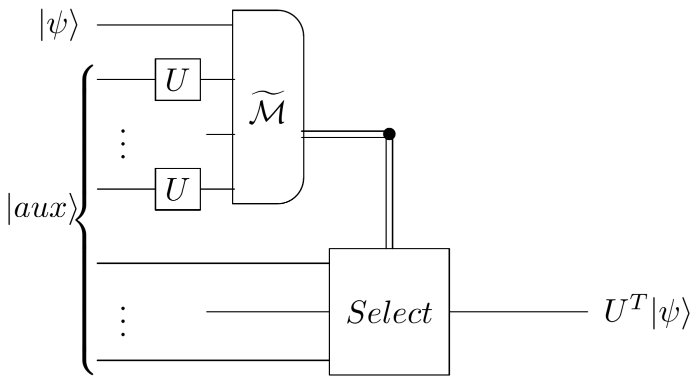


Figure 2.5: The quantum circuit for unitary transposition based on port-based teleportation. Depending on the measurement outcome of $\widetilde{\mathcal{M}}$, a selecting operation is performed to choose one quantum system and trace out the remaining.

this SDP, namely,

$$p_{opt} = 1 - \frac{d^2 - 1}{K + d^2 - 1} = 1 - O(1/K). \tag{2.53}$$

This success probability is achievable with a modified version of the port-based teleportation [52, 53] as the quantum circuit shown in Fig. 2.5.

The original port-based teleportation is given by the quantum circuit shown in Fig. 2.5 without the unitary operations denoted by U. Like the usual quantum teleportation, an entangled state $|aux\rangle$ is required as a resource, and a measurement $\widetilde{\mathcal{M}}$ is performed on the composite system of the input state $|\psi\rangle$ and a part of $|aux\rangle$. The difference between the usual quantum teleportation and the port-based teleportation is the correction part, while in the usual quantum teleportation, a certain unitary operation depending on the measurement outcome is applied to the rest of $|aux\rangle$ for correction, it is replaced by a selecting operation in the port-based teleportation, that is, all but one system of $|aux\rangle$ is traced out, and the remaining system is in the state $|\psi\rangle$. Due to the simple structure of the correction part, the port-based teleportation cannot be achieved in a deterministic and exact manner, and the port-based teleportation used here is a probabilistic one. On the other hand, since the correction part is given by a selecting operation, it commutes with any operation in the sense that $\widetilde{\mathcal{U}} \circ \text{Select} = \text{Select} \circ \widetilde{\mathcal{U}}^{\otimes K}$ holds. Moreover, as the entangled state $|aux\rangle$ satisfies $(U^{\otimes K} \otimes I)|aux\rangle = (I \otimes (U^T)^{\otimes K})|aux\rangle$ similar to the maximally entangled state, we can see that the quantum circuit shown in Fig. 2.5 performs the unitary transposition.

For unitary inversion, while the optimal success probability is not yet known, its upper bound can be obtained [14]. Assume that it is possible to perform unitary inversion with success probability p with K uses of the input operations, then it is also possible to perform unitary transposition with success probability p with $K(d-1)$ uses of the input operations by a concatenation of unitary inversion and unitary conjugation. Since the optimal success probability for unitary transposition is given by Eq. (2.53), we obtain an upper bound for the success probability of unitary inversion as

$$p_{opt} \leq 1 - \frac{d^2-1}{K(d-1)+d^2-1} = 1 - O(1/K). \tag{2.54}$$

2.6.2 Sequential Strategy

Next, we focus on the unitary inversion with sequential uses of input operations [13]. Since a parallel strategy can always be a sequential one, a higher success probability is expected and the gap between two strategies is a theoretically and practically important problem. In Ref. [13], a quantum algorithm for unitary inversion with sequential uses of the input operation is proposed. The algorithm utilizes a repeat-until-success strategy, that is, it is an algorithm that repeats a certain subroutine until it succeeds. For simplicity, we only consider the two-dimensional unitary inversion here. The subroutine is given by the quantum circuit shown in Fig. 2.6. The subroutine is similar to the quantum teleportation, which generates the state $X^i Z^j|\psi\rangle$ before correction, where $|\psi\rangle$ is the initial state and $(i,j) = (0,0),(0,1),(1,0),(1,1)$ is the outcome of the Bell measurement. For the two-dimensional unitary inversion shown in Fig. 2.6, we obtain $U^{-1}X^iZ^j|\psi\rangle$ with a single use of U by a small modification to the quantum teleportation protocol. This subroutine successfully achieves unitary inversion if $(i,j) = (0,0)$, which occurs with probability $p = 1/4$. When it fails, we can obtain the initial state $|\psi\rangle$ by applying $(X^iZ^j)^{-1}U$ with an extra use of U. Since the initial state $|\psi\rangle$ remains when it fails, we can repeat this subroutine until it succeeds.

The success probability of this algorithm scales as

$$p = 1 - \left(1 - \frac{1}{4}\right)^{\lfloor \frac{K+1}{2} \rfloor} = 1 - O(c^K) \tag{2.55}$$

where c is a constant. While this algorithm is not the optimal one for unitary inversion with sequential uses, it is enough to show that there exists an exponential gap between the parallel strategy and the sequential strategy.

The optimal success probability for unitary inversion with sequential uses is obtained numerically using SDP [13] for some d and K. For $d = 2$, the optimal

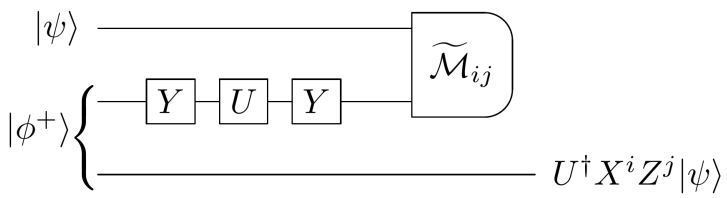


Figure 2.6: The quantum circuit for a subroutine for unitary inversion proposed in Ref. [13]. The input state is $|\psi\rangle$ and the auxiliary system is set to be the maximally entangled state $|\phi^+\rangle$. The measurement $\widetilde{\mathcal{M}}_{ij}$ is given by the Bell measurement. If the measurement outcome is $(i, j) = (0, 0)$, the inverse $U^\dagger$ is successfully obtained. Otherwise, $(X^i Z^j)^{-1} U$ is applied by an extra use of U, and the initial state $|\psi\rangle$ is recovered, which allows another repetition of this subroutine.

success probability is given by $0.4286 \simeq 3/7$ for $K = 2$ and $0.7500 \simeq 3/4$ for $K = 3$. This success probability indicates that the quantum circuit presented in Fig. 2.6 is, in fact, not the optimal one. However, the optimal supermap obtained by this SDP always assumes that we use all possible K copies of the input operation, whereas the one presented in Fig. 2.6 uses less than K copies of the input operation on average. In particular, the expected number of uses to implement the algorithm presented by Fig. 2.6 converges to finite.

Chapter 3

The Uniqueness of Quantum Switch

Quantum switch [27] is a higher-order quantum operation transforming a pair of input unitary operations into a superposition of two differently ordered concatenations of the pair of the input unitary operations. It is an example of quantum control of causal orders, and has been shown to provide some computational advantage on certain tasks such as discriminating quantum channels [31, 32, 46] and enhancing communications [33–36, 47, 48]. When two unitary operations U_1 and U_2 are given as input operations, a quantum switch transforms them into a controlled unitary operation given by

$$W = |0\rangle\langle 0| \otimes U_2 U_1 + |1\rangle\langle 1| \otimes U_1 U_2 \tag{3.1}$$

by using each of U_1 and U_2 only once. While the action of quantum switch for unitary operations is defined in a natural way, its action for general quantum operations is not trivial from the definition for unitary operations. In Ref. [27], it has been shown that one possible definition that coincides with the definition for unitary operations can be given as follows: given two quantum operations represented by the Kraus operators $\{K_i\}_i$ and $\{L_j\}_j$ respectively, the output operation of quantum switch is given by the Kraus operators $\{W_{ij}\}_{ij}$ defined by

$$W_{ij} := |0\rangle\langle 0| \otimes L_j K_i + |1\rangle\langle 1| \otimes K_i L_j. \tag{3.2}$$

Following this definition, many researches have been pursued. One interesting result is that quantum switch can help in enhancing communication tasks [33–35]. In particular, if two input operations are the depolarizing channels, which does not transfer any information, the output operation is not depolarizing channel anymore, and can be used for transferring information as stated in Sec. 2.5.2.

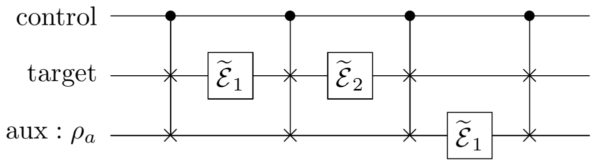


Figure 3.1: A "quantum switch" with two input operations $\widetilde{\mathcal{E}}_1$ and $\widetilde{\mathcal{E}}_2$ which uses $\widetilde{\mathcal{E}}_1$ twice. If both input operations are unitary operations, the output operation is the same as Eq. (3.1). Otherwise, the output operation may be different from the usual quantum switch of which action is given by Eq. (3.2)

The action of quantum switch on the depolarizing channels looks different from that on unitary operations, that is, coherently controlled two differently causally ordered operations, since a composition of two depolarizing channels is a depolarizing channel.

Can we assume that the action of quantum switch on general quantum operations is different from the one defined by Eq. (3.2)? Actually, it is possible if we are allowed to use the same input operation twice, for example. That is, assume the two input operations are given by $\widetilde{\mathcal{E}}_1$ and $\widetilde{\mathcal{E}}_2$, and we are allowed to use $\widetilde{\mathcal{E}}_1$ twice. In this case, it is possible to construct a "quantum switch" of which action on unitary operations does not change, but its action on the depolarizing channels is different from Eq. (2.46) as we show in the following. The assumption that quantum switch only uses the two input operations $\widetilde{\mathcal{E}}_1$ and $\widetilde{\mathcal{E}}_2$ once is important for it to be a higher-order quantum operation with indefinite causal order. In addition, we show that this assumption is necessary if we consider its action on general quantum operations beyond unitary operations.

3.1 The Uniqueness of Quantum Switch

In this chapter, we derive the suitable action of quantum switch on arbitrary quantum operations from its action on unitary operations.

We first present an example of a "quantum switch" of which action on the depolarizing channels is different from Eq. (2.46) by using the same input operation twice. Consider the quantum circuit shown in Fig. 3.1. If both input operations are unitary operations U_1 and U_2 on a d-dimensional system, the output operation is given by Eq. (3.1). Consider the case when both input operations are the depolarizing channel $\widetilde{\mathcal{D}}$, of which Kraus operators are given by $\{\frac{1}{d}U_i\}_{i=0}^{d^2-1}$ where $\{U_i\}_{i=0}^{d^2-1}$ is a set of unitary operators satisfying $\operatorname{Tr} U_i U_j^\dagger = d\delta_{ij}$ such as the generalized Pauli operators using the clock and shift operators. Similarly to Sec. 2.5.2, we assume the control qubit is in $\sqrt{p}|0\rangle + \sqrt{1-p}|1\rangle$, the target system is given by ρ, and the auxiliary system is given by ρ_a, then the action of the output operation on this input state is calculated as

$$\begin{aligned}
&\frac{1}{d^6}\sum_{i,j,k}[p|0\rangle\langle 0| \otimes U_j U_i \rho U_i^\dagger U_j^\dagger \times \operatorname{Tr} U_k \rho_a U_k^\dagger \\
&\qquad + (1-p)|1\rangle\langle 1| \otimes U_k U_j \rho U_j^\dagger U_k^\dagger \times \operatorname{Tr} U_i \rho_a U_i^\dagger \\
&\qquad + \sqrt{p(1-p)}|0\rangle\langle 1| \otimes U_j U_i \rho U_j^\dagger U_k^\dagger \times \operatorname{Tr} U_k \rho_a U_i^\dagger + h.c.] \\
&= (p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1|) \otimes \frac{I}{d} + \frac{\sqrt{p(1-p)}}{d^3}(|0\rangle\langle 1| \otimes \rho_a \rho + |1\rangle\langle 0| \otimes \rho \rho_a), \quad (3.3)
\end{aligned}$$

which is different from Eq. (2.46).

As shown in the example above, it is not possible to uniquely derive the action on arbitrary quantum operations from its action on unitary operations without further assumption. Here we introduce two extra but natural assumptions. Let $\widetilde{\widetilde{\widetilde{\mathcal{W}}}}$ be the supermap of quantum switch and W be the corresponding Choi operator. The first assumption is that quantum switch uses each input operation only once, which is equivalent to that this higher-order quantum operation is linear in each input operation. That is, the supermap $\widetilde{\widetilde{\widetilde{\mathcal{W}}}}$ satisfies

$$\begin{aligned}
&\widetilde{\widetilde{\widetilde{\mathcal{W}}}}(\alpha_1 \widetilde{\mathcal{A}}_1 + \alpha_2 \widetilde{\mathcal{A}}_2, \beta_1 \widetilde{\mathcal{B}}_1 + \beta \widetilde{\mathcal{B}}_2) \\
&\quad = \alpha_1\beta_1 \widetilde{\widetilde{\widetilde{\mathcal{W}}}}(\widetilde{\mathcal{A}}_1, \widetilde{\mathcal{B}}_1) + \alpha_1\beta_2 \widetilde{\widetilde{\widetilde{\mathcal{W}}}}(\widetilde{\mathcal{A}}_1, \widetilde{\mathcal{B}}_2) + \alpha_2\beta_1 \widetilde{\widetilde{\widetilde{\mathcal{W}}}}(\widetilde{\mathcal{A}}_2, \widetilde{\mathcal{B}}_1) + \alpha_2\beta_2 \widetilde{\widetilde{\widetilde{\mathcal{W}}}}(\widetilde{\mathcal{A}}_2, \widetilde{\mathcal{B}}_2)
\end{aligned} \quad (3.4)$$

for arbitrary complex numbers $\alpha_1, \alpha_2, \beta_1, \beta_2$ and input operations $\widetilde{\mathcal{A}}_1, \widetilde{\mathcal{A}}_2, \widetilde{\mathcal{B}}_1, \widetilde{\mathcal{B}}_2$. The second assumption is that quantum switch is described by a completely CP preserving supermap, which is equivalent to the positivity of the corresponding Choi operator $W \geq 0$. This condition is a necessary condition for the supermap to be physically implementable. We prove that under these two assumptions, the action of quantum switch can be uniquely determined from its action on only unitary operations.

Since the Choi-Jamiołkowski isomorphism is a bijection, we prove the uniqueness of the extension of quantum switch by proving that the corresponding Choi operator W is uniquely determined. Let the Hilbert spaces $\mathcal{I}_k, \mathcal{O}_k = \mathbb{C}^d$ for $k = 1, 2$ be the Hilbert spaces of the two input operations, and $\mathcal{P}, \mathcal{F} = \mathbb{C}^{2d}$ be the Hilbert spaces of the output operation as Fig. 3.2 shows. Note that $\mathcal{P}, \mathcal{F}$ can be further divided as $\mathcal{P} = \mathcal{P}_C \otimes \mathcal{P}_T$ and $\mathcal{F}_C \otimes \mathcal{F}_T$, where $\mathcal{P}_C, F_C = \mathbb{C}^2$ corresponds to the control qubit, and $\mathcal{P}_T, \mathcal{F}_T = \mathbb{C}^d$ corresponds to the target system. Let $\mathcal{H}_{in} = \mathcal{I}_1 \otimes \mathcal{O}_1 \otimes \mathcal{I}_2 \otimes \mathcal{O}_2$ and $\mathcal{H}_{out} = \mathcal{P}_T \otimes \mathcal{F}_T \otimes \mathcal{P}_C \otimes \mathcal{F}_C$. The

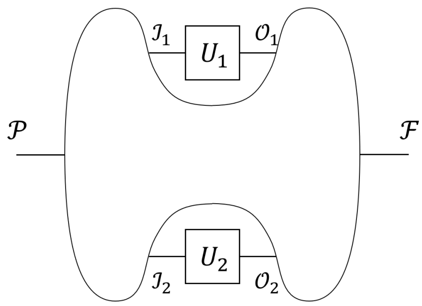


Figure 3.2: The conceptual figure of higher-order quantum operation with indefinite causal order such as quantum switch. A quantum switch takes unitary operations as input operations, and output a controlled unitary operation on Hilbert spaces $\mathcal{P}, \mathcal{F}$. The output unitary operation cannot be implemented by using the two input unitary operations in a certain order with each unitary operation used only once.

Choi operator of quantum switch W is an operator on $\mathcal{L}(\mathcal{H}_{in} \otimes \mathcal{H}_{out})$. Note that the Choi operator is define on this Hilbert space because of the assumption of linearity. We also denote the Choi operator of quantum switch defined by the Kraus operators given in Ref. [27] as $W_0 \in \mathcal{L}(\mathcal{H}_{in} \otimes \mathcal{H}_{out})$. This operator can be calculated as $W_0 = |W_0\rangle\langle W_0|$ with

$$\begin{aligned}|W_0\rangle =& |00\rangle_{\mathcal{P}_C\mathcal{F}_C} |I\rangle\rangle_{\mathcal{P}_T\mathcal{I}_1} |I\rangle\rangle_{\mathcal{O}_1\mathcal{I}_2} |I\rangle\rangle_{\mathcal{O}_2\mathcal{F}_T} \\ &+ |11\rangle_{\mathcal{P}_C\mathcal{F}_C} |I\rangle\rangle_{\mathcal{P}_T\mathcal{I}_2} |I\rangle\rangle_{\mathcal{O}_2\mathcal{I}_1} |I\rangle\rangle_{\mathcal{O}_1\mathcal{F}_T} \\ =& \sum_{i,j,k=0}^{d-1} (|ijjkik00\rangle + |jkijik11\rangle), \end{aligned} \tag{3.5}$$

where the Hilbert spaces for the vector in the last line is in the order of $\mathcal{I}_1 \otimes \mathcal{O}_1 \otimes \mathcal{I}_2 \otimes \mathcal{O}_2 \otimes \mathcal{P}_T \otimes \mathcal{F}_T \otimes \mathcal{P}_C \otimes \mathcal{F}_C$. Note that the normalization of the Choi operators is given by $\mathrm{Tr}W = \mathrm{Tr}W_0 = 2d^3$, and each elements of the matrix W_0 is 0 or 1.

In this chapter, we show that the only possible W satisfies $W = W_0$ under the following assumptions. When input operations are unitary operations denoted by $J = J_{U_1} \otimes J_{U_2}$, the action of quantum switch is given by W_0 as $\mathrm{Tr}_{in} W_0 J^t$, where the partial trace is on $\mathcal{H}_{in}$. The first assumption is that quantum switch uses each input operation only once, which is equivalent to the linearity. This assumption is automatically satisfied by using the Choi operator defined on $\mathcal{H}_{in} \otimes \mathcal{H}_{out}$. The second assumption is the positivity given by $W \geq 0$. To summarize, the uniqueness of quantum switch is formally given by Theorem 3.1.

Theorem 3.1. *Let $W_0 = |W_0\rangle\langle W_0|$ where $|W_0\rangle$ is defined by Eq. (3.5). If there exists $W \geq 0$ such that $\mathrm{Tr}_{in}[W(J_{U_1} \otimes J_{U_2})^t] = \mathrm{Tr}_{in}[W_0(J_{U_1} \otimes J_{U_2})^t]$ holds for all U_1 and U_2, then $W = W_0$ holds.*

The proof of Theorem 3.1 is given in the following sections.

3.2 The Linear Span of Unitary Operations

While the positivity is a key feature for seeking the unique extension of quantum switch, we first focus on the linearity in this section. From the linearity, the action on any input operations that is a linear combination of unitary operations is given in the same way, that is, for any $J \in \mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$ where

$$\mathrm{span}\{J_{U_1} \otimes J_{U_2}\} := \{O \mid O = \sum_{i_1,i_2} c_{i_1 i_2}(J_{U_{i_1}} \otimes J_{U_{i_2}}), c_{i_1 i_2} \in \mathbb{C}\}, \tag{3.6}$$

the action of quantum switch on J is given by $\mathrm{Tr}_{in} W_0 J^t$. For that, we consider the operators in $\mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$. Since $\mathrm{span}\{J_{U_1} \otimes J_{U_2}\} = \mathrm{span}\{J_U\} \otimes \mathrm{span}\{J_U\}$ holds, it is enough to consider the operators in $\mathrm{span}\{J_U\}$.

We first summarize the results in this section: the following operators are in $\mathrm{span}\{J_U\}$.

1. $|ii\rangle\langle jj|, |ij\rangle\langle ji| \in \mathrm{span}\{J_U\}$ for $i \neq j$.
2. $|ij\rangle\langle i'j'| \in \mathrm{span}\{J_U\}$ for $i \neq j \neq i' \neq j'$ (all of them are different).
3. $|ij\rangle\langle i'j'| \in \mathrm{span}\{J_U\}$ if only two of i, j, i', j' are the same and others are different.
4. $\sum_{j=i+k} |ij\rangle\langle ij| \in \mathrm{span}\{J_U\}$ for $k = 0, \ldots, d-1$.
5. $(|ij\rangle\langle ii| - |jj\rangle\langle ji|), (|ji\rangle\langle ii| - |jj\rangle\langle ij|) \in \mathrm{span}\{J_U\}$ for $i \neq j$.

The proof is given in Lemmas 3.1-3.5.

We remark that the set of the operators listed here do not span the whole space of $\mathrm{span}\{J_U\}$ unless $d = 2$. There are only $2d(d-1) + d(d-1)(d-2)(d-3) + 6d(d-1)(d-2) + d + 2d(d-1) = d(d^3 - 3d + 3)$ elements here, but the dimension of $\mathrm{span}\{J_U\}$ is $(d^2-1)^2 + 1$ (see Lemma C.3), which is strictly greater than $d(d^3 - 3d + 3)$ for $d > 2$. As we will show in Sec. 3.3 that Theorem 3.1 can be proved by only considering the action of quantum switch on these operators, requiring the action of quantum switch on all unitary operations is not necessary in general to uniquely determine the action of quantum switch on general quantum operations. Instead, requiring the action of quantum switch on a restricted set of unitary operations is enough for uniquely determining the action on the rest of unitary operations and general quantum operations.

Another important fact is that the action of quantum switch on the depolarizing channels is determined only by the linearity, because

$$\frac{I}{d} \otimes \frac{I}{d} \in \mathrm{span}\{J_{U_1} \otimes J_{U_2}\} \tag{3.7}$$

holds, where $\frac{I}{d}$ is the Choi operator of the depolarizing channel. This is also obvious because the depolarizing channel is a probabilistic mixture of uniformly random unitary operations. Thus, the results of Refs. [33–35] can be obtained with only the assumption of the linearity. In contrast, if we apply quantum switch to general quantum operations, the action may not be determined from only the linearity.

Lemma 3.1. *$|ii\rangle\langle jj|, |ij\rangle\langle ji| \in \mathrm{span}\{J_U\}$ holds for $i \neq j$.*

Proof. (The same Lemma is proved in Ref. [17]) Since only the linear span is considered, we use unnormalized quantum states for convenience. Consider the following maximally entangled state

$$|\psi_{\theta,\phi}\rangle = |ii\rangle + e^{i\theta}|jj\rangle + e^{i\phi}|KK\rangle, \tag{3.8}$$

where $|KK\rangle := \sum_{k\neq i,j} |kk\rangle$, then $|\psi_{\theta,\phi}\rangle\langle\psi_{\theta,\phi}| = J_U$ for some U and $|\psi_{\theta,\phi}\rangle\langle\psi_{\theta,\phi}| \in \mathrm{span}\{J_U\}$. Since

$$\begin{aligned} |\psi_{\theta,\phi}\rangle\langle\psi_{\theta,\phi}| &= |ii\rangle\langle ii| + |jj\rangle\langle jj| + |KK\rangle\langle KK| && (3.9)\\ &+ e^{-i\theta}|ii\rangle\langle jj| + e^{-i\phi}|ii\rangle\langle KK| + e^{i(\theta-\phi)}|jj\rangle\langle KK| && (3.10)\\ &+ e^{i\theta}|jj\rangle\langle ii| + e^{i\phi}|KK\rangle\langle ii| + e^{-i(\theta-\phi)}|KK\rangle\langle jj|, && (3.11) \end{aligned}$$

we obtain

$$\int_0^{2\pi} d\theta \int_0^{2\pi} d\phi \; e^{i\theta}|\psi_{\theta,\phi}\rangle\langle\psi_{\theta,\phi}| = |ii\rangle\langle jj| \in \mathrm{span}\{J_U\} \tag{3.12}$$

for all $i \neq j$. The same calculation with the maximally entangled state

$$|\psi'_{\theta,\phi}\rangle = |ij\rangle + e^{i\theta}|ji\rangle + e^{i\phi}|KK\rangle, \tag{3.13}$$

leads to $|ij\rangle\langle ji| \in \mathrm{span}\{J_U\}$ for all $i \neq j$. □

Lemma 3.2. *$|ij\rangle\langle i'j'| \in \mathrm{span}\{J_U\}$ holds for $i \neq j \neq i' \neq j'$.*

Proof. Consider the maximally entangled state

$$|\psi_{\theta,\phi}\rangle = |ij\rangle + e^{i\theta}|i'j'\rangle + e^{i\phi}|KK\rangle \tag{3.14}$$

where $|KK\rangle := |ji\rangle + |j'i'\rangle + \sum_{k\neq i,j,i'j'}|kk\rangle$. Then the same calculation of Lemma 3.1 proves $|ij\rangle\langle i'j'| \in \mathrm{span}\{J_U\}$. □

Lemma 3.3. *$|ij\rangle\langle i'j'| \in \mathrm{span}\{J_U\}$ holds if only two of i, j, i', j' are the same and others are different.*

Proof. There are 6 cases that only two of i, j, i', j' are the same and others are different. If $|ij\rangle\langle i'j'| \in \mathrm{span}\{J_U\}$, then the conjugate transpose also satisfies $|i'j'\rangle\langle ij| \in \mathrm{span}\{J_U\}$. Thus, it is enough to consider the following four cases with $i \neq j \neq k$.

$$|ii\rangle\langle jk| \in \mathrm{span}\{J_U\} \tag{3.15}$$

$$|ij\rangle\langle jk| \in \mathrm{span}\{J_U\} \tag{3.16}$$

$$|ij\rangle\langle ik| \in \mathrm{span}\{J_U\} \tag{3.17}$$

$$|ij\rangle\langle kj| \in \mathrm{span}\{J_U\} \tag{3.18}$$

For each of them, consider the following maximally entangled states, and the same calculation of Lemma 3.1 proves that they are in $\mathrm{span}\{J_U\}$, respectively.

1. $|\psi_{\theta,\phi}\rangle = |ii\rangle + e^{i\theta}|jk\rangle + e^{i\phi}|LL\rangle$ with $|LL\rangle := |kj\rangle + \sum_{l\neq i,j,k}|ll\rangle$.
2. $|\psi_{\theta,\phi}\rangle = |ij\rangle + e^{i\theta}|jk\rangle + e^{i\phi}|LL\rangle$ with $|LL\rangle := |ki\rangle + \sum_{l\neq i,j,k}|ll\rangle$.
3. $|\psi_{\theta,\phi}\rangle = |i\rangle(|j\rangle + e^{i\theta}|k\rangle) + e^{i\phi}|LL\rangle$ with $|LL\rangle := |j\rangle(|j\rangle - e^{i\theta}|k\rangle) + |ki\rangle + \sum_{l\neq i,j,k}|ll\rangle$.
4. $|\psi_{\theta,\phi}\rangle = (|i\rangle + e^{i\theta}|k\rangle)|j\rangle + e^{i\phi}|LL\rangle$ with $|LL\rangle := (|i\rangle - e^{i\theta}|k\rangle)|i\rangle + |jk\rangle + \sum_{l\neq i,j,k}|ll\rangle$.

□

Lemma 3.4. $\sum_{j=i+k}|ij\rangle\langle ij| \in \mathrm{span}\{J_U\}$ *holds for $k = 0, \ldots, d-1$.*

Proof. Consider the maximally entangled state

$$|\psi_{\theta_i}\rangle = \sum_i e^{\theta_i}|i, i+k\rangle. \tag{3.19}$$

Note that we consider the d-dimensional system and $|i+k\rangle$ indicates $|i+k \pmod{d}\rangle$. Then we obtain

$$\int_0^{2\pi}\prod_i d\theta_i\ |\psi_{\theta_i}\rangle\langle\psi_{\theta_i}| = \sum_i |i, i+k\rangle\langle i, i+k| = \sum_{j=i+k}|ij\rangle\langle ij| \in \mathrm{span}\{J_U\}. \tag{3.20}$$

□

Lemma 3.5. $(|ij\rangle\langle ii| - |jj\rangle\langle ji|), (|ji\rangle\langle ii| - |jj\rangle\langle ij|) \in \mathrm{span}\{J_U\}$ *holds for* $i \neq j$.

Proof. Consider the maximally entangled state

$$|\psi^1_{\theta,\phi}\rangle = (|i\rangle + e^{i\theta_2}|j\rangle)(|i\rangle + e^{i\theta_2}|j\rangle) + e^{i\theta_1}(|i\rangle - e^{i\theta_2}|j\rangle)(|i\rangle - e^{i\theta_2}|j\rangle) + e^{i\phi}|KK\rangle \tag{3.21}$$

$$|\psi^2_{\theta,\phi}\rangle = (|i\rangle + e^{i\theta_2}|j\rangle)(|i\rangle - e^{i\theta_2}|j\rangle) + e^{i\theta_1}(|i\rangle - e^{i\theta_2}|j\rangle)(|i\rangle + e^{i\theta_2}|j\rangle) + e^{i\phi}|KK\rangle \tag{3.22}$$

where $|KK\rangle := \sum_{k\neq i,j}|kk\rangle$. Here

$$\int_0^{2\pi} d\theta_1 d\theta_2 d\phi e^{i\theta_1} e^{-i\theta_2} |\psi^1_{\theta,\phi}\rangle\langle\psi^1_{\theta,\phi}| = |ij\rangle\langle ii| + |ji\rangle\langle ii| - |jj\rangle\langle ij| - |jj\rangle\langle ji| \tag{3.23}$$

$$\int_0^{2\pi} d\theta_1 d\theta_2 d\phi e^{i\theta_1} e^{-i\theta_2} |\psi^2_{\theta,\phi}\rangle\langle\psi^2_{\theta,\phi}| = -|ij\rangle\langle ii| + |ji\rangle\langle ii| - |jj\rangle\langle ij| + |jj\rangle\langle ji|, \tag{3.24}$$

holds, and by considering the sum and difference, we obtain

$$(|ij\rangle\langle ii| - |jj\rangle\langle ji|), (|ji\rangle\langle ii| - |jj\rangle\langle ij|) \in \mathrm{span}\{J_U\}. \tag{3.25}$$

□

3.3 The Proof of Theorem 3.1

The Choi operator W_0 of quantum switch that we prove is given by Eq. (3.5). For $J = |ijkl\rangle\langle i'j'k'l'| \in \mathcal{L}(\mathcal{I}_1 \otimes \mathcal{O}_1 \otimes \mathcal{I}_2 \otimes \mathcal{O}_2)$, the action of W_0 can be evaluated as

$$\begin{aligned} \mathrm{Tr}_{in}(W_0 J^t) &= \langle ijkl||W_0\rangle\langle W_0||i'j'k'l'\rangle & (3.26)\\ &= (\delta_{jk}|il00\rangle + \delta_{il}|kj11\rangle)(\delta_{j'k'}\langle i'l'00| + \delta_{i'l'}\langle k'j'11|) & (3.27)\\ &= \delta_{jk}\delta_{j'k'}|il00\rangle\langle i'l'00| + \delta_{il}\delta_{i'l'}|kj11\rangle\langle k'j'11| \\ &\quad + \delta_{jk}\delta_{i'l'}|il00\rangle\langle k'j'11| + \delta_{il}\delta_{j'k'}|kj11\rangle\langle i'l'00|. & (3.28) \end{aligned}$$

Note that for $J \in \mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$, $\mathrm{Tr}_{in}(WJ^t) = \mathrm{Tr}_{in}(W_0 J^t)$ holds by assumption.

Each element of W_0 is 0 or 1. In order to prove Theorem 3.1, it is enough to prove that each element of W satisfies $|(W)_{ij}| = 0$ or 1. This is because if an arbitrary extension W satisfies $|(W)_{ij}| = 0$ or 1 but $W \neq W_0$, then some elements of $\epsilon W + (1-\epsilon)W_0$, which is also a candidate for W, must have values between 0 and 1, which contradicts with the assumption that arbitrary extension W satisfies $|(W)_{ij}| = 0$ or 1.

The rest of the proof is divided into two parts: the first part considers the diagonal elements of W, and the second part considers the off-diagonal elements of W.

(First part: diagonal elements of W) Consider $J = |ijkl\rangle\langle i'j'k'l'|$, for all i, j, k, l, there exist i', j', k', l' such that $J \in \mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$. That is, if $i = j$ then let $i' = j'(\neq i)$ so that $|ij\rangle\langle i'j'| \in \mathrm{span}\{J_U\}$, and in this case, we relabel the variables i', j' as j. Similarly, if $i = j$ then let $i' = j, j' = i$ so that $|ij\rangle\langle i'j'| \in \mathrm{span}\{J_U\}$. (See Sec. 3.2) The same arguments hold for k, l. We then obtain the followings for $i \neq j$ and $k \neq l$:

$$\widetilde{\mathcal{W}}(|ijkl\rangle\langle jilk|) = (\delta_{jk}|il00\rangle + \delta_{il}|kj11\rangle)(\delta_{il}\langle jk00| + \delta_{jk}\langle li11|) \tag{3.29}$$
$$\widetilde{\mathcal{W}}(|ijkk\rangle\langle jill|) = (\delta_{jk}|ik00\rangle + \delta_{ik}|kj11\rangle)(\delta_{il}\langle jl00| + \delta_{jl}\langle li11|) \tag{3.30}$$
$$\widetilde{\mathcal{W}}(|iikl\rangle\langle jjlk|) = (\delta_{ik}|il00\rangle + \delta_{il}|ki11\rangle)(\delta_{jl}\langle jk00| + \delta_{jk}\langle lj11|) \tag{3.31}$$
$$\widetilde{\mathcal{W}}(|iikk\rangle\langle jjll|) = (\delta_{ik}|ik00\rangle + \delta_{ik}|ki11\rangle)(\delta_{jl}\langle jl00| + \delta_{jl}\langle lj11|), \tag{3.32}$$

where $\widetilde{\mathcal{W}}$ denotes the corresponding map of W, i.e., $\widetilde{\mathcal{W}}(J) = \mathrm{Tr}_{in} W J^t$. Also, consider that $I \otimes I \in \mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$, we obtain

$$\mathrm{Tr}\,\widetilde{\mathcal{W}}(I \otimes I) = \mathrm{Tr}(\mathrm{Tr}_{in} W) = \mathrm{Tr} W = 2d^3. \tag{3.33}$$

By considering Eqs. (3.29) – (3.33) and the positivity $W \geq 0$, we obtain the following elements of W with $i \neq j, k \neq l$

$$\langle ijklil00|W|ijklil00\rangle = 1 \text{ for } j = k \tag{3.34}$$
$$\langle ijklkj11|W|ijklkj11\rangle = 1 \text{ for } i = l \tag{3.35}$$
$$\langle ijkkik00|W|ijkkik00\rangle = 1 \text{ for } j = k \tag{3.36}$$
$$\langle ijkkkj11|W|ijkkkj11\rangle = 1 \text{ for } i = k \tag{3.37}$$
$$\langle iiklil00|W|iiklil00\rangle = 1 \text{ for } i = k \tag{3.38}$$
$$\langle iiklki11|W|iiklki11\rangle = 1 \text{ for } i = l \tag{3.39}$$
$$\langle iikkik00|W|iikkik00\rangle = 1 \text{ for } i = k \tag{3.40}$$
$$\langle iikkki11|W|iikkki11\rangle = 1 \text{ for } i = k, \tag{3.41}$$

or equivalently,

$$\langle ijjlil00|W|ijjlil00\rangle = 1 \text{ for } i \neq j, j \neq l \tag{3.42}$$
$$\langle ijkikj11|W|ijkikj11\rangle = 1 \text{ for } i \neq j, k \neq i \tag{3.43}$$
$$\langle ijjjij00|W|ijjjij00\rangle = 1 \text{ for } i \neq j \tag{3.44}$$
$$\langle ijiiij11|W|ijiiij11\rangle = 1 \text{ for } i \neq j \tag{3.45}$$
$$\langle iiilil00|W|iiilil00\rangle = 1 \text{ for } i \neq l \tag{3.46}$$
$$\langle iikiki11|W|iikiki11\rangle = 1 \text{ for } i \neq k \tag{3.47}$$
$$\langle iiiiii00|W|iiiiii00\rangle = 1 \tag{3.48}$$
$$\langle iiiiii11|W|iiiiii11\rangle = 1. \tag{3.49}$$

The proof is given in the rest of this part. The number of terms in 1st, 3rd, 5th and 7th lines (or 2nd, 4th, 6th, 8th lines) is given by $d(d-1)^2, d(d-1), d(d-1), d$ respectively, and the total number of terms in these 8 lines is $2d^3$. Since $\operatorname{Tr} W = 2d^3$, all the other diagonal terms of W is 0, that is, $\langle\psi|W|\psi'\rangle = 0$ for all $|\psi\rangle, |\psi'\rangle$ not of these forms.

Remark 3.1. Before providing the proof of the first part, we show how we can obtain the diagonal elements of W from Eqs. (3.29) – (3.33) and the positivity $W \geq 0$ with a simpler example. Consider a linear map $\widetilde{\mathcal{W}} : \mathcal{L}(\mathbb{C}^2) \to \mathcal{L}(\mathbb{C}^2)$ and the corresponding Choi operator $W \in \mathcal{L}(\mathbb{C}^4)$ satisfying

$$\widetilde{\mathcal{W}}(|i\rangle\langle j|) = |i\rangle\langle j| \quad \text{for} \quad (i,j) = (0,1),(1,0) \tag{3.50}$$
$$\operatorname{Tr} W = 2 \tag{3.51}$$
$$W \geq 0, \tag{3.52}$$

then the matrix W can be assumed to be

$$W = \begin{pmatrix} a & b & 0 & 1 \\ c & d & 0 & 0 \\ 0 & 0 & e & f \\ 1 & 0 & g & h \end{pmatrix} \tag{3.53}$$

with $a + d + e + h = 2$. From the positivity $W \geq 0$, we obtain $ah - 1 \geq 0$ and $a, d, e, h \geq 0$. Here the inequality

$$2 = a + d + e + h \geq 2\sqrt{ah} + e + h \geq 2 \times 1 + 0 + 0 = 2 \tag{3.54}$$

holds, and by considering the condition for the equality, we obtain $a+d = 2\sqrt{ad}$ as a necessary condition. Thus, we obtain $a = d = 1$ and the diagonal terms are uniquely determined as $(a, d, e, h) = (1, 0, 0, 1)$.

Now we provide the proof of Eqs. (3.34) – (3.41) from Eqs. (3.29) – (3.33) and the positivity $W \geq 0$. Let

$$S_1 = \{|ijklil00\rangle \mid i \neq j, k \neq l, j = k\} \cup \{|ijklkj11\rangle \mid i \neq j, k \neq l, i = l\} \quad (3.55)$$

$$S_2 = \{|ijkkik00\rangle \mid i \neq j, j = k\} \quad (3.56)$$

$$S_3 = \{|ijkkkj11\rangle \mid i \neq j, i = k\} \quad (3.57)$$

$$S_4 = \{|iiklil00\rangle \mid k \neq l, i = k\} \quad (3.58)$$

$$S_5 = \{|iiklki11\rangle \mid k \neq l, i = l\} \quad (3.59)$$

$$S_6 = \{|iikkik00\rangle \mid i = k\} \quad (3.60)$$

$$S_7 = \{|iikkki11\rangle \mid i = k\}, \quad (3.61)$$

and it is enough to prove that

$$\prod_{|\psi\rangle \in S_a} \langle\psi|W|\psi\rangle \geq 1 \quad (3.62)$$

holds for $a = 1, \ldots, 7$. This is because if Eq. (3.62) holds, the inequality

$$2d^3 \geq \sum_{a=1}^{7} \sum_{|\psi\rangle \in S_a} \langle\psi|W|\psi\rangle \geq \sum_{a=1}^{7} |S_a| \left(\prod_{|\psi\rangle \in S_a} \langle\psi|W|\psi\rangle \right)^{\frac{1}{|S_a|}} \geq \sum_{a=1}^{7} |S_a| = 2d^3 \quad (3.63)$$

also holds, and by considering the condition for the equality, we obtain

$$\langle\psi|W|\psi\rangle = 1 \quad (3.64)$$

for all $|\psi\rangle \in S_a$ for all a. Here we only prove Eq. (3.62) for $a = 1, 2, 6$. The case of $a = 4$ can be proved in the same way as the case of $a = 2$ by considering the symmetry between the two input operations. The rest cases $a = 3, 5, 7$ can be proved in the same way as $a = 2, 4, 6$, respectively, by considering the symmetry between the action of the control qubit being 0 and 1.

(Case 1: S_1) In this case, we show the following inequality holds

$$\begin{aligned} \prod_{|\psi\rangle \in S_1} \langle\psi|W|\psi\rangle &= \left(\prod_{i\neq j, k\neq l, j=k} \langle ijklil00|W|ijklil00\rangle \right) \left(\prod_{i\neq j, k\neq l, i=l} \langle ijklkj11|W|ijklkj11\rangle \right) \\ &= \left(\prod_{i\neq k, k\neq l} \langle ikklil00|W|ikklil00\rangle \right) \left(\prod_{i\neq k, k\neq l} \langle kilkli11|W|kilkli11\rangle \right) \\ &= \prod_{i\neq k, k\neq l} \langle ikklil00|W|ikklil00\rangle \langle kilkli11|W|kilkli11\rangle \geq 1. \end{aligned} \quad (3.65)$$

Let $|\psi^0_{ikl}\rangle := |ikklil00\rangle$ and $|\psi^1_{ikl}\rangle := |kilkli11\rangle$, then $\langle\psi^0_{ikl}|W|\psi^1_{ikl}\rangle = 1$ holds for arbitrary i, k, l satisfying $i \neq k, k \neq l$ because of Eq. (3.29). By considering the positivity of the submatrix

$$\begin{pmatrix} \langle\psi^0_{ikl}|W|\psi^0_{ikl}\rangle & \langle\psi^0_{ikl}|W|\psi^1_{ikl}\rangle \\ \langle\psi^1_{ikl}|W|\psi^0_{ikl}\rangle & \langle\psi^1_{ikl}|W|\psi^1_{ikl}\rangle \end{pmatrix} = \begin{pmatrix} \langle\psi^0_{ikl}|W|\psi^0_{ikl}\rangle & 1 \\ 1 & \langle\psi^1_{ikl}|W|\psi^1_{ikl}\rangle \end{pmatrix} \geq 0, \quad (3.66)$$

we obtain the inequality

$$\langle\psi^0_{ikl}|W|\psi^0_{ikl}\rangle\langle\psi^1_{ikl}|W|\psi^1_{ikl}\rangle \geq 1, \quad (3.67)$$

which completes the proof of Eq. (3.65).

(Case 2: S_2) In this case, we show the following inequality holds

$$\begin{aligned} \prod_{|\psi\rangle\in S_3} \langle\psi|W|\psi\rangle &= \prod_{i\neq j, j=k} \langle ijkkik00|W|ijkkik00\rangle \\ &= \prod_{i\neq k}\langle\psi_{ik}|W|\psi_{ik}\rangle = \prod_{i<k}\langle\psi_{ik}|W|\psi_{ik}\rangle\langle\psi_{ki}|W|\psi_{ki}\rangle \geq 1, \end{aligned} \quad (3.68)$$

where we define $|\psi_{ik}\rangle := |ikkkik00\rangle$ for $i, k = 0, \ldots, d-1$. Since $\langle\psi_{ik}|W|\psi_{ki}\rangle = 1$ holds arbitrary i, k satisfying $i \neq k$ because of Eq. (3.30), we consider the positivity of the submatrix

$$\begin{pmatrix} \langle\psi_{ik}|W|\psi_{ik}\rangle & \langle\psi_{ik}|W|\psi_{ki}\rangle \\ \langle\psi_{ki}|W|\psi_{ik}\rangle & \langle\psi_{ki}|W|\psi_{ki}\rangle \end{pmatrix} = \begin{pmatrix} \langle\psi_{ik}|W|\psi_{ik}\rangle & 1 \\ 1 & \langle\psi_{ki}|W|\psi_{ki}\rangle \end{pmatrix} \geq 0, \quad (3.69)$$

and obtain

$$\langle\psi_{ik}|W|\psi_{ik}\rangle\langle\psi_{ki}|W|\psi_{ki}\rangle \geq 1 \quad (3.70)$$

for any $i \neq k$, which completes the proof of Eq. (3.68).

(Case 3: S_6) In this case, we show the following inequality holds

$$\prod_{|\psi\rangle\in S_7} \langle\psi|W|\psi\rangle = \prod_{i=k}\langle iikkik00|W|iikkik00\rangle = \prod_{k}\langle kkkkkk00|W|kkkkkk00\rangle \geq 1. \quad (3.71)$$

Let $|\psi_k\rangle := |kkkkkk00\rangle$ for $k = 0, \ldots, d-1$, then $\langle\psi_k|W|\psi_{k'}\rangle = 1$ holds for $k \neq k'$ because of Eq. (3.32). By considering the positivity of the submatrix

$$\begin{pmatrix} \langle\psi_0|W|\psi_0\rangle & \langle\psi_0|W|\psi_1\rangle & \cdots & \langle\psi_0|W|\psi_{d-1}\rangle \\ \langle\psi_1|W|\psi_0\rangle & \langle\psi_1|W|\psi_1\rangle & \ddots & \langle\psi_1|W|\psi_{d-1}\rangle \\ \vdots & \ddots & \ddots & \vdots \\ \langle\psi_{d-1}|W|\psi_0\rangle & \langle\psi_{d-1}|W|\psi_1\rangle & \cdots & \langle\psi_{d-1}|W|\psi_{d-1}\rangle \end{pmatrix} \geq 0, \quad (3.72)$$

we obtain Eq. (3.71).

In total, we uniquely determined the diagonal elements of W.

(Second part: off-diagonal elements of W) Here we show that every element of W satisfies $|(W)_{ij}| = 0$ or 1. From the positivity, if a diagonal element is 0, then all the elements of that row or column is 0. Therefore, we can assume that W is given by

$$\begin{aligned}\mathrm{Tr}_{in} W J^t &= \langle ijkl||W\rangle\langle W||i'j'k'l'\rangle & (3.73)\\ &= a_{ijkli'j'k'l'}\delta_{jk}\delta_{j'k'}|il00\rangle\langle i'l'00| + b_{ijkli'j'k'l'}\delta_{il}\delta_{i'l'}|kj11\rangle\langle k'j'11| \\ &\quad + c_{ijkli'j'k'l'}\delta_{jk}\delta_{i'l'}|il00\rangle\langle k'j'11| + d_{ijkli'j'k'l'}\delta_{il}\delta_{j'k'}|kj11\rangle\langle i'l'00| & (3.74)\end{aligned}$$

with $|a_{ijkli'j'k'l'}|, |b_{ijkli'j'k'l'}|, |c_{ijkli'j'k'l'}|, |d_{ijkli'j'k'l'}| \leq 1$. (cf. Eq. (3.28)) As we mentioned, it is enough to show that all of the absolute values of them (with non vanishing kronecker delta) are 1. Considering that there are at most $(2d^3)^2$ non-zero elements, this is also equivalent to show that $||W||_1 = (2d^3)^2$, where $||W||_1$ denotes the element-wise 1-norm in this chapter (i.e. sum of absolute values of all elements in the computational basis). Since $||W||_1 \leq (2d^3)^2$ is trivial, we prove $||W||_1 \geq (2d^3)^2$ in the following.

Remark 3.2. Before proceeding to the proof, we briefly explain the key idea of the proof (by adding an extra assumption which makes the proof much simpler). Let $J = \sum_{ijkli'j'k'l'} |ijkl\rangle\langle i'j'k'l'|$, then $||W||_1 \geq ||\mathrm{Tr}_{in} W J^t||_1$ holds because of the triangle inequality. Assume that $J \in \mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$ (which is the extra assumption and is not true), then the r.h.s. can be evaluated using $\mathrm{Tr}_{in} W J^t = \mathrm{Tr}_{in} W_0 J^t$ as

$$||W||_1 \geq ||\mathrm{Tr}_{in} W J^t||_1 = ||\mathrm{Tr}_{in} W_0 J^t||_1 = (2d^3)^2, \tag{3.75}$$

which completes the proof.

In order to evaluate $||W||_1$, we first provide a grouping of $|ijkl\rangle\langle i'j'k'l'| = |ij\rangle\langle i'j'| \otimes |kl\rangle\langle k'l'|$, which covers all possible elements and also satisfies that each group is in $\mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$. See Sec. 3.2 for the proof that they are in $\mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$. We first classify $|ij\rangle\langle i'j'|$ into the following groups. (i, j, i', j' are assumed to be different by default)

1. If all i, j, i', j' are different, or if only two of them are the same, or $i = j, i' = j'$ or $i = j', j = i'$, then we use $|ij\rangle\langle i'j'| \in \mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$.

2. If $i = i', j = j'$ or $i = i' = j = j'$, then we use $\sum_{j=i+k} |ij\rangle\langle ij| \in \mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$.

3. If $i = j = j'$ or $i = j = j'$ or $i = i' = j'$ or $j = i' = j$, then we use $(|ij\rangle\langle ii| - |jj\rangle\langle ji|), (|ji\rangle\langle ii| - |jj\rangle\langle ij|) \in \mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$.

We denote the three groups as G_1, G_2 and G_3 respectively. To make the statement clear, we provide the definitions explicitly as follows:

$$
\begin{aligned}
G_1 = \{|ij\rangle\langle i'j'| \mid & \; i \neq j \neq i' \neq j', \\
& \text{or } i = j, i \neq i' \neq j' \text{ (and the remaining 5 patterns)}, \\
& \text{or } i = j, i' = j', i \neq i', \text{ or } i = j', j = i', i \neq j\}, \qquad (3.76) \\
G_2 = \{ \sum_{j=i+k} & |ij\rangle\langle ij| \mid k = 0, \ldots, d-1\}, \qquad (3.77) \\
G_3 = \{|ij\rangle\langle ii| & - |jj\rangle\langle ji|, |ji\rangle\langle ii| - |jj\rangle\langle ij| \mid i \neq j\}. \qquad (3.78)
\end{aligned}
$$

The number of elements of each group is given by

$$
\begin{aligned}
|G_1| &= d(d-1)(d-2)(d-3) + 6d(d-1)(d-2) + 2d(d-1) \qquad (3.79) \\
&= d(d-1)(d^2 + d - 4), \qquad (3.80) \\
|G_2| &= d, \qquad (3.81) \\
|G_3| &= 2d(d-1). \qquad (3.82)
\end{aligned}
$$

Note that $|G_1| + d|G_2| + 2|G_3| = d^4$ holds. The same grouping is chosen for $|kl\rangle\langle k'l'|$. By considering the triangle inequality and that the three groups has no overlap, we obtain

$$
||W||_1 \geq \sum_{a,b=1}^{3} \sum_{J \in G_a \otimes G_b} ||\mathrm{Tr}_{in} W J^t||_1. \qquad (3.83)
$$

Moreover, since all J considered here satisfies $J \in \mathrm{span}\{J_{U_1} \otimes J_{U_2}\}$, we can evaluate the r.h.s. with $\mathrm{Tr}_{in} W J^t = \mathrm{Tr}_{in} W_0 J^t$.

The summation $\sum_{J \in G_a \otimes G_b} ||\mathrm{Tr}_{in} W J^t||_1$ for each a, b is evaluated as follows. See Appendix A for calculations. Note that it is enough to consider only 6 cases that satisfy $a \leq b$ because of the symmetry between the two systems.

$$\sum_{J\in G_1\otimes G_1} ||\mathrm{Tr}_{in} W J^t||_1 = 2d(d-1)(2d^4 + 2d^3 - 18d^2 + 11d + 8), \tag{3.84}$$

$$\sum_{J\in G_1\otimes G_2} ||\mathrm{Tr}_{in} W J^t||_1 = 2d(d-1)(2d^2 - d - 4), \tag{3.85}$$

$$\sum_{J\in G_2\otimes G_2} ||\mathrm{Tr}_{in} W J^t||_1 = 2d^2(d+1), \tag{3.86}$$

$$\sum_{J\in G_1\otimes G_3} ||\mathrm{Tr}_{in} W J^t||_1 = 4d(d-1)(4d^2 - 5d - 2), \tag{3.87}$$

$$\sum_{J\in G_2\otimes G_3} ||\mathrm{Tr}_{in} W J^t||_1 = 4d(d-1)(d+2), \tag{3.88}$$

$$\sum_{J\in G_3\otimes G_3} ||\mathrm{Tr}_{in} W J^t||_1 = 16d^2(d-1). \tag{3.89}$$

By using these equations, $||W||_1$ is evaluated as

$$||W||_1 \geq (2d^3)^2, \tag{3.90}$$

which completes the prove of Theorem 3.1.

Chapter 4

Controlled Quantum Operations, Controlled Quantum Combs, and Controllization

A quantum version of a conditional operation is a controlled unitary operation. Even though a controlled version of a unitary operation is well-defined, it has been shown that universal controllization of unitary operations maintaining full coherence is not implementable with a single use of the unitary operation within quantum mechanics [21–24]. This no-go theorem of universal controllization of a unitary operation restricts quantum programming, since whenever the controlled unitary operation is used in a quantum algorithm, controllization has to be performed based on the description of each unitary operation. There are several preceding researches on controllization of unitary operations by relaxing the situation of the no-go theorem.

In this chapter, we analyze the problem of universal controllization as controlled higher-order quantum operations. Introduction of well-defined controlled versions of general quantum operations and higher-order quantum operations provides a novel tool for quantum programming, in addition to the standard controlled unitary operations.

In Sec. 4.1, we first seek an "appropriate" definition of a controlled general deterministic quantum operation for utilizing controlled quantum operations in quantum computation by extending the definition of controlled unitary operations. In our definition, controlled quantum operations with different degrees of coherence are defined with a Kraus operator contributing to the coherence. The coherence of a controlled quantum operation is evaluated by the trace norm of an off-diagonal term of its Choi operator. If the Hilbert-Schmidt norm of the Kraus operator contributing to the coherence is 0, it is classically controlled (no coherence), and if it is 1, it is fully coherently controlled as in the case of standard controlled unitary operations, and controlled quantum operations with intermediate coherence are also included. For each quantum operation, the maximal Hilbert-Schmidt norm of the operator is determined, which we call the most coherently controlled quantum operation. In Sec. 4.2, we discuss the relationship between quantum switch and controlled quantum operations based on our definition.

In Sec. 4.3, we further extend our definition to a controlled version of quantum combs. We then show that universal controllization can be regarded as a controlled version of a neutralization comb, a quantum comb transforming any quantum operations into the identity operation. A controlled neutralization comb can perform a transformation from a quantum operation to its controlled version, although the maximal coherence may not be guaranteed in general.

The idea of controlled neutralization comb provides a unified way of understanding and analyzing controllization. By utilizing the most coherently controlled neutralization combs, the quantum algorithms presented in Sec. 2.4 can be understood in a way as presented in Sec. 4.4.1. We also propose a new quantum algorithm for universal controllization which can be implemented without any auxiliary system. The new algorithm for universal controllization we present in Sec. 4.4.2 and Sec. 4.4.3 is based on randomization using the Pauli operations and the Clifford operations, respectively. We evaluate both randomizations, and we show that the randomization using the Pauli operations performs better than the randomization using the Clifford operations.

4.1 Controlled Quantum Operations

4.1.1 Controlled Quantum Operations Based on Physical Implementations

We seek an appropriate definition of controlled quantum operations by generalizing the definition of the controlled unitary operations preserving coherence $J_{\mathcal{C}_U}$ instead of the incoherent version $J_{\mathcal{C}_U^{\text{cls}}}$. In this section, we consider two possible generalizations based on two different implementation schemes of controlled unitary operations, and both generalizations emerge to the same definition.

The first definition of the controlled quantum operation is based on the Stinespring representation [45] of a quantum operation, which is represented by the quantum circuit shown in Fig. 4.1. For a quantum operation $\widetilde{\mathcal{A}}$ represented by the Kraus operators given by $\{K_i\}_{i=1}^n$, it is always possible to define a unitary operator U on an extended quantum system $\mathcal{H} \otimes \mathcal{H}_{\text{aux}}$ by adding an auxiliary

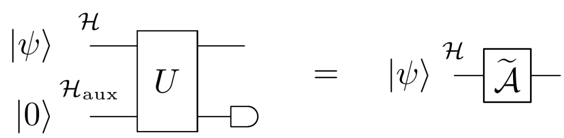


Figure 4.1: A quantum circuit for Stinespring representation of a quantum operation. A quantum operation $\widetilde{\mathcal{A}} : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{K})$ can be implemented by adding an auxiliary system $\mathcal{H}_{\text{aux}}$ in a state $|0\rangle$ to an initial state $|\psi\rangle$ on $\mathcal{H}$ and applying a unitary operation U on the joint system $\mathcal{H} \otimes \mathcal{H}_{\text{aux}}$. The unitary operator U is called purification of the Kraus operators of $\widetilde{\mathcal{A}}$.

system $\mathcal{H}_{\text{aux}} = \mathbb{C}^{n+1}$ satisfying

$$U|\psi\rangle|0\rangle = \sum_{i=1}^{n} K_i|\psi\rangle|i\rangle \tag{4.1}$$

for an arbitrary state $|\psi\rangle \in \mathcal{H}$, where $\{|i\rangle\}_{i=0}^{n}$ is an orthonormal basis of the auxiliary system. Note that we take a particular U such that the summation over i starts from 1 instead of 0 in the r.h.s. of Eq. (4.1) to treat each Kraus operator K_i for $i = 1, \ldots, n$ equally. This choice is equivalent to taking the Kraus operators $\{K_i\}_{i=0}^{n}$ with $K_0 = 0$. We call this U as a purification of the Kraus operators $\{K_i\}$. The quantum operation $\widetilde{\mathcal{A}}$ can be represented as the reduced dynamics of this unitary operation as

$$\widetilde{\mathcal{A}}(|\psi\rangle\langle\psi|) = \mathrm{Tr}_{\text{aux}}\left[U\left(|\psi\rangle\langle\psi| \otimes |0\rangle\langle 0|\right)U^{\dagger}\right]. \tag{4.2}$$

Considering the controlled unitary operation defined by Eq. (2.36), the Choi operator of the controlled unitary operation of the purification Eq. (4.1) is given by $J_{\mathcal{C}_U} \in \mathcal{L}(\mathcal{H}_C \otimes \mathcal{K}_C \otimes \mathcal{H} \otimes \mathcal{K} \otimes \mathcal{H}_{\text{aux}} \otimes \mathcal{K}_{\text{aux}})$ as

$$J_{\mathcal{C}_U} = \Big(|00\rangle|I\rangle\!\rangle|00\rangle + |11\rangle\sum_{i=1}^{n}|K_i\rangle\!\rangle|0i\rangle\Big)\Big(\langle 00|\langle\!\langle I|\langle 00| + \langle 11|\sum_{j=1}^{n}\langle\!\langle K_j|\langle 0j|\Big) \tag{4.3}$$

where $|mm\rangle|X\rangle\!\rangle|0n\rangle$ is a tensor product of $|mm\rangle \in \mathcal{H}_C \otimes \mathcal{K}_C$, $|X\rangle\!\rangle \in \mathcal{H} \otimes \mathcal{K}$ and $|0n\rangle \in \mathcal{H}_{\text{aux}} \otimes \mathcal{K}_{\text{aux}}$. We omitted the global phase dependence in Eq. (4.3), since it can be absorbed in the choice of the Kraus operators. By tracing out the auxiliary system $\mathcal{H}_{\text{aux}} \otimes \mathcal{K}_{\text{aux}}$, the Choi operator of the reduced dynamics is obtained as

$$\mathrm{Tr}_{\text{aux}}(J_{\mathcal{C}_U}) = |00\rangle\langle 00| \otimes J_{id} + |11\rangle\langle 11| \otimes J_{\mathcal{A}}. \tag{4.4}$$

This is the classically controlled quantum operation defined by Eq. (2.39). Even when $\widetilde{\mathcal{A}}$ is a unitary operation whose Kraus operator is given by a single element set $\{K_1 = V\}$ of a unitary operator V, the construction of the Choi operator based on Eq. (4.1) derives $J_{\mathcal{C}_U^{\mathrm{cls}}}$ instead of $J_{\mathcal{C}_U}$ which preserves coherence.

The loss of coherence here originates from ignoring the freedom in the purification of the identity operation applied in the case that the control qubit is $|0\rangle$. In other words, there is an asymmetry that the identity operation is implemented without purification while $\widetilde{\mathcal{A}}$ is. The general form of the Kraus operators of the identity operation is given as $\{K_i = \alpha_i I\}$ satisfying $\sum_i |\alpha_i|^2 = 1$. The corresponding purification U_0 of these Kraus operators of the identity operation is given by

$$U_0|\psi\rangle|0\rangle = |\psi\rangle \sum_{i=1}^{n} \alpha_i |i\rangle. \tag{4.5}$$

Here U_0 is a unitary operator acting non-trivially only on the auxiliary system $\mathcal{H}_{\mathrm{aux}}$. We consider that U_0 is applied when the control qubit is $|0\rangle$ instead of I on $\mathcal{H} \otimes \mathcal{H}_{\mathrm{aux}}$ in the controlled quantum operation. Then the corresponding unitary operator of the controlled operation $\widetilde{\mathcal{C}}_{U,U_0}$ is

$$C_{U,U_0} = |0\rangle\langle 0| \otimes U_0 + |1\rangle\langle 1| \otimes U. \tag{4.6}$$

The corresponding Choi operator is given as

$$J_{\mathcal{C}_{U,U_0}} = \sum_{i,j=1}^{n} \Big(\alpha_i |00\rangle|I\rangle\rangle + |11\rangle|K_i\rangle\rangle\Big)\Big(\alpha_j^* \langle 00|\langle\langle I| + \langle 11|\langle\langle K_j|\Big) \otimes |0i\rangle\langle 0j|, \tag{4.7}$$

By tracing out the auxiliary system $\mathcal{H}_{\mathrm{aux}} \otimes \mathcal{K}_{\mathrm{aux}}$, we obtain

$$\mathrm{Tr}_{\mathrm{aux}} J_{\mathcal{C}_{U,U_0}} = \sum_{i} \Big(\alpha_i |00\rangle|I\rangle\rangle + |11\rangle|K_i\rangle\rangle\Big)\Big(\alpha_i^* \langle 00|\langle\langle I| + \langle 11|\langle\langle K_i|\Big). \tag{4.8}$$

The corresponding quantum circuit is shown in Fig. 4.2. We take the definition given by Eq. (4.8) as the first definition of a controlled quantum operation. For a given quantum operation, controlled quantum operations with different degrees of coherence can be defined by changing the set of Kraus operators $\{K_i\}$ and coefficients $\{\alpha_i\}$.

In the appendix of Ref. [49], a definition of a controlled quantum operation is introduced in terms of purification with an environment. They obtained a similar representation of ours where $\alpha_i = \langle i|U_0|0\rangle$ in Eq. (4.8) is given by $\langle i|\varepsilon_0\rangle$ with an initial state of the environment $|\varepsilon_0\rangle$ in their definition. The main difference between the definition of Ref. [49] and our definition is that we explicitly choose a certain type of Kraus operators $\{K_i\}_{i=0}^{n}$ satisfying $K_0 = 0$. By this choice of the Kraus operators and the corresponding purification U, the quantum circuit

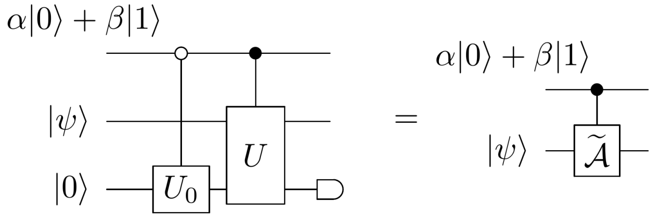
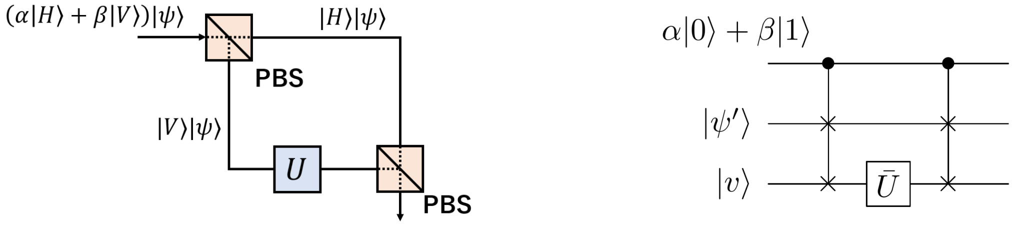


Figure 4.2: A definition of controlled quantum operation based on the Stinespring representation. There is extra freedom by introducing U_0 applied to the auxiliary system depending on the state of the control qubit, which can be regarded as a purification of the identity operation. Given a fixed U, controlled quantum operations with all possible degrees of coherence for a given quantum operation $\widetilde{\mathcal{A}}$ are implementable by only changing U_0.

shown in Fig. 4.2 can implement controlled quantum operations with all possible degrees of coherence by just choosing the coefficients $\{\alpha_i\}$ or equivalently U_0. We will analyze this point at the end of Sec. 4.1.2.

The second definition of a controlled quantum operation is to use an additional dimension, based on the implementation of a controlled unitary operation in the optical interferometer system [22, 23, 30, 54, 55]. Consider a composite of quantum states of the control qubit $\alpha|0\rangle + \beta|1\rangle$ and the target state $|\psi\rangle$. We assume that the control qubit and the target state are encoded into the a single photon. That is, the control qubit is encoded into the polarization of a photon as $\alpha|H\rangle + \beta|V\rangle$, where $|H\rangle$ and $|V\rangle$ denote the horizontal and the vertical polarization, and the target state is encoded into other degrees of freedom of the same photon such as the orbital angular momentum or the transverse spatial mode, which is represented by the Hilbert space $\mathcal{H}$. A unitary operation represented by $U \in \mathcal{L}(\mathcal{H})$ can be realized by an optical element which acts on the addition degrees of freedom but not the polarization, and the corresponding controlled unitary operation $\widetilde{\mathcal{C}}_U$ can be implemented with the optical interferometer shown in Fig. 4.3a. The polarization of the photon controls its path via polarization beam splitters, and the optical elements corresponding to U is placed in the lower path. If the polarization of the photon is in $|V\rangle$, the photon pass through the lower path and U is applied on the target state $|\psi\rangle$. If the polarization of the photon is in $|H\rangle$, the photon pass through the upper path, and the vacuum state pass through the optical elements corresponding to U which remains to be the vacuum state. Thus, the resulting quantum state is given by $\alpha|H\rangle|\psi\rangle + \beta|V\rangle U|\psi\rangle$, and the action of the controlled unitary operation is obtained. By considering the vacuum state $|v\rangle$, which is ignored in the formulation of optical elements, a unitary operation U on the Hilbert space $\mathcal{H}$



(a) (b)

Figure 4.3: (a) An implementation of a controlled unitary operation in an optical interferometer [22, 23]. The optical element PBS denotes a polarization beam splitter, and the polarization $|H\rangle$ and $|V\rangle$ control the routing of the optical path. The lower path has an optical element acting on the additional degrees of freedom, which corresponds to the unitary operation U acting on the target system. (b) An equivalent quantum circuit to the optical interferometer by introducing the vacuum state $|v\rangle$. The control qubit $|0\rangle$ and $|1\rangle$ correspond to the polarization $|H\rangle$ and $|V\rangle$. The target state $|\psi'\rangle$ is a quantum state embedded in a one-dimension larger Hilbert space $|\psi'\rangle \in \mathcal{H}\oplus\mathbb{C}$ that is equivalent to the original target state $|\psi\rangle \in \mathcal{H}$ as $|\psi'\rangle = |\psi\rangle + 0|v\rangle$. The auxiliary state is given by the vacuum state $|v\rangle \in \mathcal{H}\oplus\mathbb{C}$, and the unitary operation $\bar{U} = U \oplus |v\rangle\!\langle v| \in \mathcal{L}(\mathcal{H}\oplus\mathbb{C})$ does not change the vacuum state $|v\rangle$.

can be regarded as a unitary operation $\bar{U}$ embedded into a one-dimension larger Hilbert space $\mathcal{H} \oplus \mathbb{C}$ as $\bar{U} = U \oplus |v\rangle\!\langle v|$. The optical interferometer shown in Fig. 4.3a with the unitary operation U can be regarded as the quantum circuit shown in Fig. 4.3b with the unitary operation $\bar{U}$.

An embedded unitary operation $\bar{U}$ is transformed to the corresponding controlled unitary operation $\widetilde{\mathcal{C}}_{\bar{U}}$ by the optical interferometer shown in Fig. 4.3. This transformation is represented by the following function f, namely,

$$
\begin{aligned}
f(J_{\bar{U}}) &= |00\rangle\!\langle 00| \otimes J_{\bar{id}} + |11\rangle\!\langle 11| \otimes J_{\bar{U}} + |00\rangle\!\langle 11| \otimes |\bar{I}\rangle\!\rangle\!\langle\!\langle \bar{U}| + h.c. &\quad (4.9)\\
&= |00\rangle\!\langle 00| \otimes J_{\bar{id}} + |11\rangle\!\langle 11| \otimes J_{\bar{U}} + |00\rangle\!\langle 11| \otimes |\bar{I}\rangle\!\rangle(\langle vv|J_{\bar{U}}) + h.c., &\quad (4.10)
\end{aligned}
$$

where $|\bar{U}\rangle\!\rangle = |U\rangle\!\rangle + |vv\rangle$ by definition of the embedded space, and the second equality holds because of $\langle vv|\bar{U}\rangle\!\rangle = 1$. Note that the function f only depends on $J_{\bar{U}}$, which is uniquely determined for a unitary operation.

This optical interferometer implementation for a controlled unitary operation can also be extended for general quantum operations. A quantum operation $\widetilde{\mathcal{A}}$ can be extended to $\widetilde{\bar{\mathcal{A}}}$ of a larger dimensional system by extending the Kraus operators as $\bar{K}_i = K_i \oplus \alpha_i|v\rangle\!\langle v|$, where coefficients $\{\alpha_i\}$ satisfying $\sum_i |\alpha_i|^2 = 1$ are necessary so that $\{\bar{K}_i\}$ is also a Kraus representation of a quantum operation.

For a quantum operation given by the Kraus operators $\{\bar{K}_i\}$, the controlled version given by the optical interferometer shown in Fig. 4.3 is uniquely determined by the Choi operator $f(J_{\bar{\mathcal{A}}})$ as

$$f(J_{\bar{\mathcal{A}}}) = |00\rangle\langle 00| \otimes J_{\bar{id}} + |11\rangle\langle 11| \otimes J_{\bar{\mathcal{A}}} + |00\rangle\langle 11| \otimes |\bar{I}\rangle\rangle(\langle vv|J_{\bar{\mathcal{A}}}) + h.c. \quad (4.11)$$

$$= \sum_i (\alpha_i|00\rangle|I\rangle\rangle + |11\rangle|K_i\rangle\rangle + \alpha_i|\xi\rangle|vv\rangle)$$
$$\times (\alpha_i^*\langle 00|\langle\langle I| + \langle 11|\langle\langle K_i| + \alpha_i^*\langle\xi|\langle vv|), \quad (4.12)$$

where $|\xi\rangle = |00\rangle + |11\rangle$ is a vector in $\mathcal{H}_C \otimes \mathcal{K}_C$. Assuming that the input state of this extended operation does not contain the vacuum state, that is, it is orthogonal to $|\psi_{\text{ctrl}}\rangle|v\rangle$, where $|\psi_{\text{ctrl}}\rangle$ is an arbitrary state of the control qubit, the third term in each bracket does not affect the result, and Eq. (4.12) is equivalent to Eq. (4.8).

The two different definitions emerge to the identical one given by

$$J_{\mathcal{C}_{\mathcal{A}}^{K_i,\alpha_i}} = \sum_i \Big(\alpha_i|00\rangle|I\rangle\rangle + |11\rangle|K_i\rangle\rangle\Big)\Big(\alpha_i^*\langle 00|\langle\langle I| + \langle 11|\langle\langle K_i|\Big). \quad (4.13)$$

We stress that a characteristic property of this definition of a controlled quantum operation $J_{\mathcal{C}_{\mathcal{A}}^{K_i,\alpha_i}}$ is that it cannot be uniquely determined by the Choi operator $J_{\mathcal{A}}$, but depends on both the choice of the Kraus operators $\{K_i\}$ and the coefficients $\{\alpha_i\}$. This is in contrast to the classical controlled version of a quantum operation $J_{\mathcal{C}_{\mathcal{A}}^{\text{cls}}}$, which is uniquely determined for $\widetilde{\mathcal{A}}$.

4.1.2 Axiomatic Definition of Controlled Quantum Operations

In this section, we define a controlled quantum operation in an axiomatic manner. We show that we can derive the definition of the form given in Eq. (4.13) from a small number of axioms. We consider that a controlled quantum operation should satisfy the following three criteria.

Axiom 4.1 (Axioms for controlled quantum operations)**.** *The action of a controlled quantum operation of a deterministic quantum operation $\widetilde{\mathcal{A}}$ satisfies the following three axioms.*

1. *If the state of the control qubit is $|0\rangle$ or $|1\rangle$, the state of the control qubit remains unchanged after applying the controlled quantum operation.*

2. *If the state of the control qubit is $|0\rangle$, the identity operation is applied to the target system.*

3. If the state of the control qubit is $|1\rangle$, the quantum operation $\widetilde{\mathcal{A}}$ is applied to the target system.

The form of the controlled quantum operation given by Eq. (4.13) can be derived from just these three axioms as follows. A general form of the Kraus operators of a quantum operation on a composite system consisting of a control system and a target system is written by

$$\begin{aligned} L_i &= |0\rangle\langle 0| \otimes A_i + |0\rangle\langle 1| \otimes B_i + |1\rangle\langle 0| \otimes C_i + |1\rangle\langle 1| \otimes D_i \\ &\in \mathcal{L}(\mathcal{H}_C \otimes \mathcal{H}, \mathcal{K}_C \otimes \mathcal{K}) \end{aligned} \tag{4.14}$$

Due to the first axiom, terms in L_i that change the control qubit state must vanish as $B_i = C_i = 0$. To satisfy the second axiom, each A_i must be proportional to identity, that is, $A_i = \alpha_i I$ with $\sum_i |\alpha_i|^2 = 1$ is required. The third axiom implies that $\{D_i\}$ is a Kraus representation of $\widetilde{\mathcal{A}}$. Therefore, the Kraus operator of the controlled quantum operation has to be in a form of

$$L_i = \alpha_i |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes K_i, \tag{4.15}$$

where $\sum_i |\alpha_i|^2 = 1$ and $\{K_i\}$ is a Kraus representation of $\widetilde{\mathcal{A}}$. The quantum operation given by the Kraus operators $\{L_i\}$ is equivalent to that of Eq. (4.13).

A controlled quantum operation is characterized by the parameters $\{\alpha_i\}$ and $\{K_i\}$, but not all different combinations of these correspond to all different controlled quantum operations in general, namely, these parameters are redundant. In the following, we provide a parameterization that uniquely determines a controlled quantum operation. By expanding Eq. (4.13), we obtain

$$J_{\mathcal{C}_{\mathcal{A}}^{K_i,\alpha_i}} = J_{\mathcal{C}_{\mathcal{A}}^{\text{cls}}} + |00\rangle\langle 11| \otimes |I\rangle\rangle\langle\langle K| + |11\rangle\langle 00| \otimes |K\rangle\rangle\langle\langle I|, \tag{4.16}$$

where $J_{\mathcal{C}_{\mathcal{A}}^{\text{cls}}}$ is a controlled quantum operation of $\widetilde{\mathcal{A}}$ without coherence defined by Eq. (2.39) and K is the operator given by $K = \sum_i \alpha_i^* K_i$. As a Choi operator uniquely determines a quantum operation, the operator K fully specifies one controlled quantum operation of $\widetilde{\mathcal{A}}$ without redundancy. Note that the operator K corresponds to the transformation matrix introduced in Ref. [49]. In the following, we use the definition of the controlled quantum operation $\widetilde{\mathcal{C}}_{\mathcal{A}}^{K}$ for $\widetilde{\mathcal{A}}$ with a choice of $K = \sum_i \alpha_i^* K_i$ for $\widetilde{\mathcal{A}}$ as

$$J_{\mathcal{C}_{\mathcal{A}}^{K}} := J_{\mathcal{C}_{\mathcal{A}}^{\text{cls}}} + |00\rangle\langle 11| \otimes |I\rangle\rangle\langle\langle K| + |11\rangle\langle 00| \otimes |K\rangle\rangle\langle\langle I|. \tag{4.17}$$

Now we show that the quantum circuit shown in Fig. 4.2 can implement controlled quantum operations with all possible degrees of coherence for a given quantum operation by choosing only the coefficients $\{\alpha_i\}$ or equivalently U_0. More precisely, given a fixed set of Kraus operators $\{K_i\}_{i=0}^n$ with $K_0 = 0$, for any set of the Kraus operators $\{K'_j\}_{j=0}^m$ with $K'_0 = 0$ and coefficients $\{\alpha'_j\}_{j=0}^m$ with $\sum_j |\alpha'_j|^2 = 1$, we can choose $\{\alpha_i\}$ with $\sum_i |\alpha_i|^2 = 1$ to make the two resulting controlled quantum operations to be equivalent. This property implies that we can represent all possible controlled quantum operations for a given quantum operation by any choice of the Kraus operators with our definition given by Eq. (4.8).

Since $\{K_i\}_{i=0}^n$ and $\{K'_j\}_{j=0}^m$ represent the same quantum operation, $K'_j = \sum_i u^*_{ji} K_i$ holds with a unitary matrix (u_{ij}). Note that if $n \neq m$, we pad with $K_i, K'_j = 0$ to make the number of the Kraus operators to be the same. In order to implement the controlled quantum operation with $K = \sum_j (\alpha'_j)^* K'_j$, by considering $\sum_j (\alpha'_j)^* K'_j = \sum_{i,j=0}^n (\alpha'_j)^* u^*_{ji} K_i$, we can choose $\alpha_i = \sum_j \alpha'_j u_{ji}$ when the Kraus operators are given by $\{K_i\}_{i=0}^n$. For $n < m$, $\sum_{i=0}^n |\alpha_i|^2$ may be smaller than 1, we pad $\{K_i\}_{i=0}^n$ to $\{K_i\}_{i=0}^m$ with $K_i = 0$ for $n < i \leq m$. However, since we assumed $K_0 = 0$, we can re-define the coefficient $|\alpha_0|^2$ by $|\alpha_0|^2 + \sum_{i=n+1}^m |\alpha_i|^2$ to satisfy $\sum_{i=0}^n |\alpha_i|^2 = 1$. Note that the phase of α_0 can be chosen arbitrarily as the corresponding Kraus operator is $K_0 = 0$. For $n \geq m$, $\sum_{i=0}^n |\alpha_i|^2 = 1$ is satisfied by construction. Thus, for a given set of the Kraus operators $\{K_i\}_{i=0}^n$ with $K_0 = 0$, we can choose only the coefficients $\{\alpha_i\}$ to define controlled quantum operations with all possible degrees of coherence, and it also indicates that the quantum circuit shown in Fig. 4.2 can be used to implement corresponding all possible controlled quantum operations.

4.1.3 Most Coherently Controlled Quantum Operation

The controlled quantum operation defined by $\widetilde{\mathcal{C}}_{\mathcal{A}}^K$ contains different types of controlled quantum operations including the classically controlled version of quantum operations depending on the choice of K. However, in quantum information processing, keeping coherence or superposition of states is important. Thus, we consider a characterization of the most coherently controlled quantum operation in this section.

Since we focus on the coherence between the different states of the control qubit, we investigate the (block) off-diagonal term of the corresponding Choi operator of a controlled quantum operation. Especially, we consider the off-diagonal term of the Choi operator indicating coherence of a controlled quantum operation given by

$$\Delta J_{\mathcal{C}_{\mathcal{A}}^K} = J_{\mathcal{C}_{\mathcal{A}}^K} - J_{\mathcal{C}_{\mathcal{A}}^{\mathrm{cls}}}. \tag{4.18}$$

The trace norm of $\Delta J_{\mathcal{C}_{\mathcal{A}}^{K}}$ corresponds to a distance measure between quantum operations [56]. We regard that the controlled quantum operation that has the largest norm of the off-diagonal term, which can be also interpreted to be the most distant one from the classically controlled version, as the quantum mechanically most coherent one. Here $\Delta J_{\mathcal{C}_{\mathcal{A}}^{K}}$ has only two non-zero eigenvalues $\lambda = \pm\sqrt{d}\sqrt{\mathrm{Tr}\,[K^\dagger K]}$ and the corresponding two eigenstates are given by $(1/\sqrt{d})|00\rangle \otimes |I\rangle\rangle \pm (1/\sqrt{\mathrm{Tr} K^\dagger K})|11\rangle \otimes |K\rangle\rangle$. Thus, we obtain the Schatten p-norm[1] of this operator $||X||_p = \sqrt[p]{\mathrm{Tr}\,[|X|^p]}$ as

$$\left|\left|\Delta J_{\mathcal{C}_{\mathcal{A}}^{K}}\right|\right|_p = 2^{\frac{1}{p}}\sqrt{d}\sqrt{\mathrm{Tr}\,[K^\dagger K]}. \tag{4.19}$$

According to Eq. (4.19), $\widetilde{\mathcal{C}}_{\mathcal{A}}^{K}$ with maximum quantum coherence (in the sense of the Schatten p-norm) is obtained by maximizing the Hilbert-Schmidt norm of K. In order to calculate the Hilbert-Schmidt norm, we introduce the orthogonal Kraus operators $\{\bar{K}_j\}$ as follows. For any quantum operation $\widetilde{\mathcal{A}}$, we can take a set of mutually orthogonal Kraus operators $\{\bar{K}_j\}_{j=1}^m$ satisfying $\mathrm{Tr}\,\bar{K}_i{}^\dagger \bar{K}_j = 0$ for all $i \neq j$. Explicitly, $\{\bar{K}_j\}_{j=1}^m$ can be obtained by first calculating the Choi operator of $\widetilde{\mathcal{A}}$, and then performing the spectral decomposition on the Choi operator. Note that the number of the Kraus operator in the orthogonal Kraus representation $\{\bar{K}_j\}_{j=1}^m$ satisfies $m \leq n$ where n is the number of the Kraus operators in an arbitrary Kraus representation $\{K_i\}_{i=1}^n$. We can rewrite $K = \sum_i \alpha_i^* K_i$ as $K = \sum_i \beta_i^* \bar{K}_i$ with

$$\beta_i = \frac{\mathrm{Tr}\,K^\dagger \bar{K}_i}{\mathrm{Tr}\,\bar{K}_i{}^\dagger \bar{K}_i} \tag{4.20}$$

by defining $\bar{K}_i = 0$ for $m < i \leq n$ when $m < n$. The coefficients $\{\beta_i\}$ satisfy $\sum_i |\beta_i|^2 \leq 1$ and this can be shown as follows. Since $\{K_i\}$ and $\{\bar{K}_j\}$ represent the same quantum operation, $K_i = \sum_{j=1}^n u_{ij}\bar{K}_j$ holds with a unitary matrix (u_{ij}). Then we obtain

$$\sum_{j=1}^m |\beta_i|^2 = \sum_{i,j=1}^n |\alpha_i|^2 |u_{ij}|^2 \delta_{i\leq m} = \sum_{i=1}^m |\alpha_i|^2 \leq \sum_{i=1}^n |\alpha_i|^2 = 1 \tag{4.21}$$

where $\delta_{i\leq m}$ denotes a step function, namely, $\delta_{i\leq m} = 1$ for $i \leq m$ and otherwise $\delta_{i\leq m} = 0$.

By using the orthogonal Kraus operators $\{\bar{K}_i\}$, the Hilbert-Schmidt norm of K is represented as

$$\mathrm{Tr}\,K^\dagger K = \sum_i |\beta_i|^2\, \mathrm{Tr}\,\bar{K}_i{}^\dagger \bar{K}_i, \;\; \sum_i |\beta_i|^2 \leq 1. \tag{4.22}$$

[1] The trace norm corresponds to $p = 1$.

We define a subset of the index of the orthogonal Kraus operators $\{\bar{K}_i\}$ of a quantum operation $\widetilde{\mathcal{A}}$ with the maximum Hilbert-Schmidt norm as

$$A_{\max} := \left\{ i \;\middle|\; \forall j,\ \mathrm{Tr}\,\bar{K}_i{}^\dagger \bar{K}_i \geq \mathrm{Tr}\,\bar{K}_j{}^\dagger \bar{K}_j \right\}. \tag{4.23}$$

It is clear from Eq. (4.22) that the operator K for the maximum coherence is obtained by appropriately choosing the coefficients $\{\alpha_i\}$ for the orthogonal Kraus operators with the maximum Hilbert-Schmidt norm as

$$K = \sum_{i \in A_{\max}} \alpha_i^* \bar{K}_i, \quad \sum_i |\alpha_i|^2 = 1. \tag{4.24}$$

We can construct an orthogonal Kraus representation of $\widetilde{\mathcal{A}}$ which includes K as one of the Kraus operator. In other words, K is one of the possible Kraus operators of $\widetilde{\mathcal{A}}$ which has the maximum Hilbert-Schmidt norm. In the following, we call a controlled quantum operation of $\widetilde{\mathcal{A}}$ described with the maximum Hilbert-Schmidt norm of K as the *most coherently controlled quantum operation.* In particular, when the maximal Hilbert-Schmidt norm of K is 1, we refer such a controlled quantum operation to as the *fully* coherently controlled quantum operation. The controlled unitary operations given by Eq. (2.37) is the fully coherently controlled quantum operation as expected.

Remark that the definition of a controlled quantum operation can be generalized by replacing the identity operation applied when the control qubit state is $|0\rangle$ with another general quantum operation, such as the depolarizing channel. Such kinds of controlled quantum operations are considered in Ref. [49, 50]. However, it is difficult to evaluate the coherence in general for such cases, and it is not clear what can be regarded as the most coherently controlled quantum operation. Nevertheless, the most coherently controlled quantum operation can be easily extended if another quantum operation described by a single Kraus operator, e.g., an isometry V, is applied when the control qubit state is $|0\rangle$, instead of the identity operation. In this case, by replacing the identity operator by the isometry V in Eq. (4.15), all the calculation directly follows, and the eigenvalue to calculate Eq. (4.19) becomes $\pm\sqrt{\mathrm{Tr}\,[V^\dagger V]}\sqrt{\mathrm{Tr}\,[K^\dagger K]}$. Since the TP condition is given as $V^\dagger V = I$ for deterministic quantum operations, we obtain the same value of coherence as Eq. (4.19).

4.2 Relationship between Controlled Quantum Operations and Quantum Switch

Recently, the effects of a quantum switch [27] on general quantum operations have been extensively analyzed. It is reported that quantum switch enhances the communication capacity of the input channels, including the completely depolarizing channel [33, 35, 48] (Sec. 2.5). While some consider the enhancement is due to the indefinitely causally ordered aspect of quantum switch, others claim that such a phenomenon can happen in systems exploiting coherently controlled quantum operations without causally indefinite elements [49, 50]. In this section, we investigate the relationship between controlled quantum operations and quantum switch based on our definition of controlled quantum operations.

In Ref. [49], it is pointed out that the action of quantum switch on the depolarizing channels presented in Ref. [33] can be obtained by considering controlled depolarizing channels. That is, by taking $K = \frac{1}{d}I$ in our definition for controlled quantum operations, the action of concatenation of two controlled depolarizing channels (with one of them having inverted control qubit, namely, applying the depolarizing channel if control qubit is in $|1\rangle$ and do nothing if in $|0\rangle$) is equivalent to the action of quantum switch on depolarizing channels. In order to avoid confusion, we denote the controlled quantum operation of $\widetilde{\mathcal{A}}$ with inverted control qubit as $\widetilde{\mathcal{C}}^{\circ}_{\mathcal{A}}$ in this section. That is, $\widetilde{\mathcal{C}}^{\circ}_{\mathcal{A}} := \widetilde{\mathcal{X}}_c \circ \widetilde{\mathcal{C}}_{\mathcal{A}} \circ \widetilde{\mathcal{X}}_c$ where $\widetilde{\mathcal{X}}_c$ denotes the Pauli X operation (NOT operation) on the control qubit. To simplify the problem, here we consider only two-dimensional case. The Kraus operators for the depolarizing channel $\widetilde{\mathcal{D}}$ is given by $\{\frac{1}{2}\sigma_i\}_{i=0}^{3}$, where σ_i denotes the Pauli operators as $\sigma_0 = I, \sigma_1 = X, \sigma_2 = Y, \sigma_3 = Z$. The Choi operator of the output quantum operation of quantum switch is calculated as

$$\begin{aligned} &|00\rangle\langle 00| \otimes \frac{I}{2} + |11\rangle\langle 11| \otimes \frac{I}{2} + |00\rangle\langle 11| \otimes \sum_{i,j} \frac{1}{2^4} |\sigma_i\sigma_j\rangle\rangle\langle\langle\sigma_j\sigma_i| + h.c. \\ &= |00\rangle\langle 00| \otimes \frac{I}{2} + |11\rangle\langle 11| \otimes \frac{I}{2} + (|00\rangle\langle 11| + |11\rangle\langle 00|) \otimes \frac{1}{4}|I\rangle\rangle\langle\langle I| \end{aligned} \tag{4.25}$$

by using the commutation relation of the Pauli operators. The resulting quantum operation of concatenation of two controlled depolarizing channels, $\widetilde{\mathcal{C}}^{\circ L}_{\mathcal{D}} \circ \widetilde{\mathcal{C}}^{K}_{\mathcal{D}} = \widetilde{\mathcal{C}}^{K}_{\mathcal{D}} \circ \widetilde{\mathcal{C}}^{\circ L}_{\mathcal{D}}$, is given by

$$|00\rangle\langle 00| \otimes \frac{I}{2} + |11\rangle\langle 11| \otimes \frac{I}{2} + |00\rangle\langle 11| \otimes |L\rangle\rangle\langle\langle K| + |11\rangle\langle 00| \otimes |K\rangle\rangle\langle\langle L|, \tag{4.26}$$

where K and L denotes the Kraus operators defining the controlled quantum operation. It is easy to see that the two resulting quantum operations coincide if we take $K = L = \frac{1}{2}I$ as Ref. [49] pointed out.

In Ref. [57, 58], the authors pointed out that while the input state passes through both depolarizing channels in quantum switch case, it passes through only a single depolarizing channel in the controlled depolarizing channel case. In fact, the action of both cases coincides because concatenations of depolarizing channels are depolarizing channel. Moreover, the authors pointed out that the concatenation of two controlled depolarizing channel is different from a single controlled depolarizing channel. In our formalism, this fact is also obvious. Assuming that the two depolarizing channels are characterized by K_1, K_2, then the concatenated one is characterized by K_2K_1. While K_2K_1 is a Kraus operator for the concatenated channel, such a product does not cover the whole set of Kraus operators of the concatenated channel. For example, for the depolarizing channel case, while $\frac{1}{2}I$ is a Kraus operator of a single channel, it cannot be a product of two Kraus operators of the depolarizing channel, i.e., of the form K_2K_1 with K_1, K_2 being the Kraus operators of the depolarizing channel.

In this section, we also show that if the input quantum operation is different from the depolarizing channel, such coincidence does not happen in general, not only because the concatenation of two channels is not the same as the original one, but also the coherent term cannot be the same. In particular, we consider the case where the input quantum operation $\widetilde{\mathcal{A}}$ is given by the Kraus operators $\{\alpha_i\sigma_i\}_{i=0}^3$ with $\alpha_i \geq 0$ satisfying $\sum \alpha_i^2 = 1$. Note that the depolarizing channel corresponds to $\alpha_i = 1/2$ for all i. The action of quantum switch on this quantum channel is given by

$$|00\rangle\langle 00| \otimes J_{\mathcal{A}\circ\mathcal{A}} + |11\rangle\langle 11| \otimes J_{\mathcal{A}\circ\mathcal{A}} + |00\rangle\langle 11| \otimes B + |11\rangle\langle 00| \otimes B^\dagger \tag{4.27}$$

where the off-diagonal term B is given by

$$\begin{aligned} B = \sum_i \alpha_i^4 |I\rangle\rangle\langle\langle I| + 2[(\alpha_0\alpha_1)^2 - (\alpha_2\alpha_3)^2]|X\rangle\rangle\langle\langle X| \\ + 2[(\alpha_0\alpha_2)^2 - (\alpha_1\alpha_3)^2]|Y\rangle\rangle\langle\langle Y| + 2[(\alpha_0\alpha_3)^2 - (\alpha_1\alpha_2)^2]|Z\rangle\rangle\langle\langle Z| \end{aligned} \tag{4.28}$$

On the other hand, if we consider the concatenation of two controlled versions, which are characterized by K, L, respectively, the resulting quantum operation $\widetilde{\mathcal{C}}_{\mathcal{A}}^{\circ L} \circ \widetilde{\mathcal{C}}_{\mathcal{A}}^{K}$ is given by

$$|00\rangle\langle 00| \otimes J_{\mathcal{A}} + |11\rangle\langle 11| \otimes J_{\mathcal{A}} + |00\rangle\langle 11| \otimes |L\rangle\rangle\langle\langle K| + |11\rangle\langle 00| \otimes |K\rangle\rangle\langle\langle L|. \tag{4.29}$$

Here the two operators K, L have to satisfy

$$K = \sum_i \beta_i(\alpha_i\sigma_i) \quad \sum_i |\beta_i|^2 \leq 1, \tag{4.30}$$

$$L = \sum_i \gamma_i(\alpha_i\sigma_i) \quad \sum_i |\gamma_i|^2 \leq 1, \tag{4.31}$$

and thus, we obtain

$$|L\rangle\rangle\langle\langle K| = \sum_{i,j} \gamma_i\beta_j^*\alpha_i\alpha_j|\sigma_i\rangle\rangle\langle\langle\sigma_j|. \tag{4.32}$$

From Eq. (4.28), we can see that unless $\alpha_i = 1/2$ for all i or $\alpha_i = 1$ for one i and otherwise 0, which correspond to the depolarizing channel and the Pauli operations, respectively, at least one of $|\sigma_i\rangle\rangle\langle\langle\sigma_i|$ for $i \neq 0$ remains. Assuming that $|\sigma_1\rangle\rangle\langle\langle\sigma_1|$ remains. Then, in order to let the same term in Eq. (4.32) be non-zero, it is required that $\alpha_1, \beta_1, \gamma_1 \neq 0$. Also, the term $|I\rangle\rangle\langle\langle I|$ in Eq. (4.28) is non-zero, and it is required that $\alpha_0, \beta_0, \gamma_0 \neq 0$ from Eq. (4.32). However, this indicates that the term $|\sigma_0\rangle\rangle\langle\langle\sigma_1|$ is also non-zero in Eq. (4.32), where such term does not exist in Eq. (4.28). Thus, the two resulting quantum operations can coincide only if the input operation is the depolarizing channel or the Pauli operations among the quantum operation given by the Kraus operators $\{\alpha_i\sigma_i\}_{i=0}^3$.

If we consider the controlled version of the concatenation of two channels, $\widetilde{\mathcal{C}}^{\circ L}_{\mathcal{A}\circ\mathcal{A}} \circ \widetilde{\mathcal{C}}^{K}_{\mathcal{A}\circ\mathcal{A}}$, the diagonal terms coincide, but the coherent term still cannot coincide. The concatenation of two quantum channel $J_{\mathcal{A}\circ\mathcal{A}}$ is given by $\{\alpha'_i\sigma_i\}_{i=0}^3$ where

$$\alpha'_0 = \sqrt{\sum_i \alpha_i^4} \tag{4.33}$$

$$\alpha'_1 = \sqrt{2(\alpha_0\alpha_1)^2 + 2(\alpha_2\alpha_3)^2} \tag{4.34}$$

$$\alpha'_2 = \sqrt{2(\alpha_0\alpha_2)^2 + 2(\alpha_1\alpha_3)^2} \tag{4.35}$$

$$\alpha'_3 = \sqrt{2(\alpha_0\alpha_3)^2 + 2(\alpha_1\alpha_2)^2} \tag{4.36}$$

Here the two operators K, L have to satisfy

$$K = \sum_i \beta_i(\alpha'_i\sigma_i) \quad \sum_i |\beta_i|^2 \leq 1, \tag{4.37}$$

$$L = \sum_i \gamma_i(\alpha'_i\sigma_i) \quad \sum_i |\gamma_i|^2 \leq 1, \tag{4.38}$$

and thus, we obtain

$$|L\rangle\rangle\langle\langle K| = \sum_{i,j} \gamma_i\beta_j^*\alpha'_i\alpha'_j|\sigma_i\rangle\rangle\langle\langle\sigma_j|. \tag{4.39}$$

Similarly, we can see that unless $\alpha_i = 1/2$ for all i or $\alpha_i = 1$ for one i and otherwise 0, i.e., the depolarizing channel and the Pauli operations, the two resulting quantum operations cannot coincide. Note that here the coherence between two quantum channels to be concatenated is allowed as we consider the controlled version of $\widetilde{\mathcal{A}} \circ \widetilde{\mathcal{A}}$, i.e., $\widetilde{\mathcal{C}}^{K}_{\mathcal{A}\circ\mathcal{A}}$. This also includes the case of the concatenation of two independently controlled channel, i.e., $\widetilde{\mathcal{C}}^{K_2}_{\mathcal{A}} \circ \widetilde{\mathcal{C}}^{K_1}_{\mathcal{A}}$, because if K_1 and K_2 are the Kraus operators for the quantum operation $\widetilde{\mathcal{A}}$, then it is also possible to choose $K = K_2K_1$ as a Kraus operator for $\widetilde{\mathcal{A}} \circ \widetilde{\mathcal{A}}$. The inverse is not possible in general, and unless coherent control of $\widetilde{\mathcal{D}} \circ \widetilde{\mathcal{D}}$ is allowed, the controlled depolarizing channel does not have the same action as the output operation of quantum switch, that is, there exists no K_1, K_2, L_1, L_2 such that $\widetilde{\mathcal{C}}_{\mathcal{D}}^{\circ L_2} \circ \widetilde{\mathcal{C}}_{\mathcal{D}}^{\circ L_1} \circ \widetilde{\mathcal{C}}_{\mathcal{D}}^{K_2} \circ \widetilde{\mathcal{C}}_{\mathcal{D}}^{K_1}$ coincide with Eq. (4.25).

4.3 Controlled Quantum Combs

In this section, we extend the definition of controlled quantum operations to controlled quantum supermaps, especially controlled quantum combs. We consider a quantum comb $\widetilde{\widetilde{\mathcal{S}}}$ transforming N quantum operations $\widetilde{\mathcal{A}}_k : \mathcal{L}(\mathcal{H}_{2k-1}) \to \mathcal{L}(\mathcal{H}_{2k})$ for $k = 1, \ldots, N$ to a target quantum operation $\widetilde{\mathcal{A}}_0 : \mathcal{L}(\mathcal{H}_0) \to \mathcal{L}(\mathcal{H}_{2N+1})$ as Fig. 4.4 shows. The Choi operator of this quantum comb S satisfies

$$S \geq 0 \tag{4.40}$$

$$\mathrm{Tr}_{2k+1} S^{(2k+1)} = \mathrm{Tr}_{2k,2k+1} S^{(2k+1)} \otimes \frac{I_{2k}}{d_{2k}}, \tag{4.41}$$

for $k = 0, 1, \ldots, N$ and $S^{(2k+1)} := \mathrm{Tr}_{2k+2,\ldots,2N+1} S$. While we usually use the Choi operator as a mathematical description for quantum combs, quantum combs can also be described by the Kraus operators $\{S_i\}$ as

$$\widetilde{\mathcal{S}}(J) = \sum_i S_i J S_i^\dagger, \tag{4.42}$$

with $S_i \in \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_{2N}, \mathcal{H}_0 \otimes \mathcal{H}_{2N+1})$. The Kraus representation and the Choi representation are related as

$$S = \sum_i |S_i\rangle\rangle\langle\langle S_i|. \tag{4.43}$$

Note that the condition for S_i is not $\sum_i S_i^\dagger S_i = I$, which is the condition for a quantum operation to be TP. Instead, the conditions for S_i are determined by the conditions given by Eq. (4.41). In Appendix B, we rewrite this condition in terms of the Kraus operators.

In the following, we define the controlled version of a quantum comb analogous to the case of quantum operations given by Eq. (4.17) presented in Sec. 4.1. In the definition of a controlled quantum comb, it is not straightforward to define an identity comb, which corresponds to the identity operation for defining controlled quantum operations. Here we consider the following quantum comb as the identity comb. Assuming that $\dim \mathcal{H}_{2k} = \dim \mathcal{H}_{2k+1}$, we define the identity

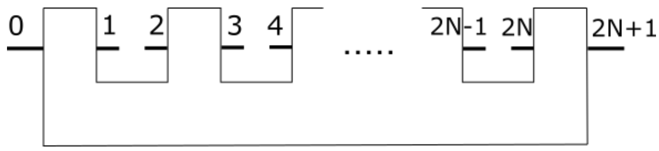


Figure 4.4: A quantum comb with N input quantum operations. The k-th input quantum operation is a quantum operation transforming a state on $\mathcal{H}_{2k-1}$ to $\mathcal{H}_{2k}$. The resulting quantum operation is a quantum operation transforming a state on $\mathcal{H}_0$ to $\mathcal{H}_{2N+1}$.

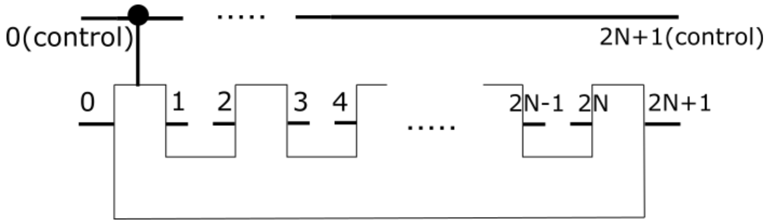


Figure 4.5: A controlled quantum comb. The initial and the final Hilbert spaces of the control system belongs to the initial and the final Hilbert spaces of the quantum comb.

comb $\widetilde{\widetilde{\mathcal{S}}}_{id}$ as a quantum comb that transfers the state in $\mathcal{H}_{2k}$ to $\mathcal{H}_{2k+1}$ without any change for all k. The action of this quantum comb is given by

$$\widetilde{\widetilde{\mathcal{S}}}_{id}(\widetilde{\mathcal{A}}_1 \otimes \cdots \otimes \widetilde{\mathcal{A}}_N) = \widetilde{\mathcal{A}}_N \circ \cdots \circ \widetilde{\mathcal{A}}_1. \tag{4.44}$$

This identity comb can also be represented as

$$\widetilde{\mathcal{S}}_{id}(J) = K_{id} J K_{id}^\dagger \tag{4.45}$$

where K_{id} is the corresponding Kraus operator given by

$$K_{id} = \left(\bigotimes_{k=0}^{N} \langle\langle I|_{2k,2k+1} \right) |I\rangle\rangle_{0,0} |I\rangle\rangle_{2N+1,2N+1}. \tag{4.46}$$

Note that the following arguments of this section can be generalized to the case that the quantum comb is described by a single Kraus operator, instead of this identity comb.

Analogous to the controlled quantum operation defined by Eq. (4.17), we define the controlled version of quantum comb $\widetilde{\widetilde{\mathcal{C}}}_{\mathcal{S}}$ as in Fig. 4.5 by the following Choi operator

$$\begin{aligned} C_{\mathcal{S}}^K := & |00\rangle\langle 00| \otimes S_{id} + |11\rangle\langle 11| \otimes S \\ & + |00\rangle\langle 11| \otimes |I\rangle\rangle\langle\langle K| + |11\rangle\langle 00| \otimes |K\rangle\rangle\langle\langle I|, \end{aligned} \tag{4.47}$$

where $K = \sum_i \alpha_i^* K_i$ with $\sum_i |\alpha_i|^2 = 1$ and S_{id} is the Choi operator of the identity comb. If we trace out the final system $\mathcal{H}_{2N+1}$, which includes the control qubit system, the third and fourth terms vanishes. Thus, it is clear if the quantum comb to be controlled satisfies the sequential condition given by Eq. (4.41), the controlled version also satisfies the same condition and is a valid quantum comb.

Moreover, as in the quantum operation case, we can define the *most coherently controlled quantum comb* in terms of the operator K by

$$K = \sum_{i \in B_{\max}} \alpha_i^* \tilde{K}_i, \quad \sum_i |\alpha_i|^2 = 1, \tag{4.48}$$

where $\{\tilde{K}_i\}$ is an orthogonal Kraus representation of the quantum comb $\widetilde{\widetilde{\mathcal{S}}}$ and

$$B_{\max} := \left\{ i \,\middle|\, \forall j,\ \operatorname{Tr} \tilde{K}_i^\dagger \tilde{K}_i \geq \operatorname{Tr} \tilde{K}_j^\dagger \tilde{K}_j \right\}. \tag{4.49}$$

4.3.1 Neutralization Comb and Controlled Quantum Operations

In this section, we investigate the relationship between controlled quantum operations and controlled quantum combs. We consider a class of quantum combs which we call *neutralization combs*, i.e., quantum combs transforming any input quantum operation into the identity operation. A quantum comb $\widetilde{\widetilde{\mathcal{N}}}$ which takes N quantum operations $\widetilde{\mathcal{A}}_1, \ldots, \widetilde{\mathcal{A}}_N$ as inputs is a neutralization comb if

$$\widetilde{\widetilde{\mathcal{N}}}(\widetilde{\mathcal{A}}_1 \otimes \cdots \otimes \widetilde{\mathcal{A}}_N) = \widetilde{id}. \tag{4.50}$$

Note that the condition given by Eq. (4.50) does not uniquely determine a neutralization comb, and there are many quantum combs satisfying Eq. (4.50) forming a class of neutralization combs.

When we have quantum operations $\widetilde{\mathcal{A}}_1, \ldots, \widetilde{\mathcal{A}}_N$ as input operations of a controlled neutralization comb, the resulting quantum operation is a controlled quantum operation of $\widetilde{\mathcal{A}}_N \circ \cdots \circ \widetilde{\mathcal{A}}_1$. That is, if the control qubit is in $|0\rangle$, the controlled quantum operation applies the identity operation, and if the control qubit is in $|1\rangle$, it applies $\widetilde{\mathcal{A}}_N \circ \cdots \circ \widetilde{\mathcal{A}}_1$. (See Axiom 4.1) From now on, for adopting the standard notation of controlled quantum operations, we exchange the state of the control qubit when the identity comb is applied and when a neutralization comb is applied. Namely, we apply the neutralization comb if the control qubit is in $|0\rangle$ and apply the identity comb if the control qubit is in $|1\rangle$, so that the role of the control qubit of the resulting controlled quantum operation coincides with the standard definition of controlled quantum operations.

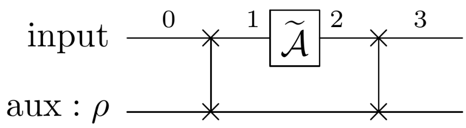


Figure 4.6: A neutralization comb with a single input quantum operation $\widetilde{\mathcal{A}}$ defined by Eq. (4.51) with $N = 1$. Any input state of $\mathcal{H}_0$ is sent to the output state without any change regardless of the quantum operation $\widetilde{\mathcal{A}}$.

One way to implement a neutralization comb is to apply the input quantum operations on the auxiliary system, and then discarding the auxiliary system. Mathematically, this neutralization comb is described as

$$N = |I\rangle\!\rangle\langle\!\langle I|_{0,2N+1} \otimes \rho_{\mathcal{H}_{in}} \otimes I_{\mathcal{H}_{out}}, \tag{4.51}$$

where $\mathcal{H}_{in} = \bigotimes_{k=1}^{N} \mathcal{H}_{2k-1}, \mathcal{H}_{out} = \bigotimes_{k=1}^{N} \mathcal{H}_{2k}$ and $\rho \in \mathcal{L}(\mathcal{H}_{in})$ is a quantum state that is initially prepared in the auxiliary system. The corresponding quantum circuit of this neutralization comb for $N = 1$ is shown in Fig. 4.6.

It would be the first guess to simply use this neutralizing comb for defining a most coherently controlled neutralization comb and then obtain the most coherently controlled quantum operation. However, the most coherently controlled neutralization comb does not necessarily provide the most coherently controlled quantum operation in general. For example, consider the neutralization comb given by Eq. (4.51) for $N = 1$. When $\widetilde{\mathcal{A}}$ is a single unitary operation described by U, the corresponding most coherently controlled operation is given by the controlled unitary operation C_U defined as Eq. (2.35). However, it is shown that the controlled unitary operation is not implementable in this situation [21–24], regardless of how the controlled neutralization comb is defined.

While universal controllization is not possible in this case, the most coherently controlled neutralization comb can implement the action of the most coherently controlled quantum operation by restricting the set of the input quantum operations. One example of such a restricted set is the set of unitary operations of which one of the eigenstates of the unitary operator U is given, that is, $\{U \mid U|\psi\rangle = e^{i\theta_U}|\psi\rangle\}$ where $|\psi\rangle$ is an eigenstate and θ_U is an arbitrary phase. Note that the implementation of a controlled unitary operation in the optical interferometer system (Fig. 4.3) can be regarded as a special case where the eigenstate $|\psi\rangle$ is given by the vacuum state $|v\rangle$.

Consider the controlled neutralization comb given by Eq. (4.51). It is easy to see that if we set the auxiliary state to be $\rho = |\psi\rangle\langle\psi|$, the controlled unitary operation is implemented. Mathematically, this neutralization comb is described by $N = |I\rangle\!\rangle\langle\!\langle I|_{03} \otimes |\psi\rangle\langle\psi|_1 \otimes I_2$. Only the eigenvector which has the maximal norm

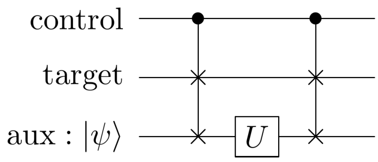


Figure 4.7: Quantum circuit for the controlled neutralization defined by Eq. (4.52). If the unitary operator U has an eigenstate $|\psi\rangle$, this quantum circuit exactly implements the corresponding controlled unitary operation.

contributes for the most coherently controlled comb. In this case, it is possible to choose any elements as $|K_0\rangle\rangle = |I\rangle\rangle_{03} \otimes |\psi\rangle_1 \otimes |\phi\rangle_2$ with an arbitrary state $|\phi\rangle$. By requiring the controlled version of the identity operation $\widetilde{id} : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{K})$ is still an identity operation $\widetilde{id} : \mathcal{L}(\mathcal{H}_C \otimes \mathcal{H}) \to \mathcal{L}(\mathcal{K}_C \otimes \mathcal{K})$, we obtain $|\phi\rangle = |\psi^*\rangle$, and the corresponding fully coherently controlled neutralization comb is given by

$$\begin{aligned} C_N &= |00\rangle\langle 00| \otimes N + |11\rangle\langle 11| \otimes |I\rangle\rangle\langle\langle I| \\ &\quad + |00\rangle\langle 11| \otimes |K_0\rangle\rangle\langle\langle I| + |11\rangle\langle 00| \otimes |I\rangle\rangle\langle\langle K_0|, \end{aligned} \tag{4.52}$$

$$|K_0\rangle\rangle = |I\rangle\rangle_{03} \otimes |\psi\rangle_1 \otimes |\psi^*\rangle_2. \tag{4.53}$$

A quantum circuit for this implementation of the neutralization comb is shown in Fig. 4.7. The action of this controlled neutralization comb C_N for U is given as

$$\begin{aligned} &\mathrm{Tr}_{\mathcal{H}_{in}\mathcal{H}_{out}}[N(|U\rangle\rangle\langle\langle U|_{12})^T] \\ &= |00\rangle\langle 00| \otimes J_{id} + |11\rangle\langle 11| \otimes J_U + |11\rangle\langle 00| \otimes \langle\langle U^*|_{12}(|I\rangle\rangle\langle\langle K_0|_{0123})|U^*\rangle\rangle_{12} + h.c. \\ &= |00\rangle\langle 00| \otimes J_{id} + |11\rangle\langle 11| \otimes J_U + |11\rangle\langle 00| \otimes |e^{-i\theta_U} U\rangle\rangle\langle\langle I|_{03} + h.c. \end{aligned} \tag{4.54}$$

where the last equality holds because of

$$\begin{aligned} \langle\langle U^*|_{12}|K_0\rangle\rangle_{0123} &= |I\rangle\rangle_{03} \sum_i \langle ii|(I \otimes U^T)|\psi\psi^*\rangle \\ &= |I\rangle\rangle_{03} \sum_i \langle ii|(U \otimes I)|\psi\psi^*\rangle \\ &= |I\rangle\rangle_{03} e^{i\theta_U}. \end{aligned} \tag{4.55}$$

4.4 Universal Controllization utilizing Controlled Neutralization Comb

4.4.1 Neutralization Comb for Multiple Copies of an Input Unitary Operation

In this section, we show that the algorithm for controllization of divisible unitary operations presented in Sec. 2.4.3 (Fig. 2.4) can be reproduced by using the idea of neutralization comb. For simplicity, we consider the case that the input unitary operation is described by a d-dimensional unitary operator U, and by using this unitary operation n times to implement the controlled quantum operation $|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U^n$. Note that in this case, the output of the identity comb is given by U^n.

We assume that the neutralization comb is achieved by preparing an auxiliary state and then tracing out the auxiliary system, which can be written as

$$N = |I\rangle\rangle\langle\langle I|_{0,2n+1} \otimes \rho_{\mathcal{H}_{in}} \otimes I_{\mathcal{H}_{out}}. \tag{4.56}$$

The controlled version of this neutralization comb is described by $|K_0\rangle\rangle = \lambda |I\rangle\rangle \otimes |\psi\rangle \otimes |\phi\rangle$ with arbitrary states $|\psi\rangle$, $|\phi\rangle$ and a normalization constant $|\lambda| \leq 1$. The action of this controlled comb is

$$\begin{aligned}\mathrm{Tr}_{\mathcal{H}_{in}\mathcal{H}_{out}}[C_N(|U\rangle\rangle\langle\langle U|^{\otimes n})^T] = |00\rangle\langle 00| \otimes J_{id} + |11\rangle\langle 11| \otimes J_{U^n} \\ + |11\rangle\langle 00| \otimes |U^n\rangle\rangle\langle\langle K_0|(|(U^*)^n\rangle\rangle) \\ + |00\rangle\langle 11| \otimes (\langle\langle (U^*)^n|)|K_0\rangle\rangle\langle\langle U^n|.\end{aligned} \tag{4.57}$$

The resulting controlled unitary operation is required to be

$$|00\rangle\langle 00| \otimes J_{id} + |11\rangle\langle 11| \otimes J_{U^n} + |11\rangle\langle 00| \otimes |U^n\rangle\rangle\langle\langle I| + |00\rangle\langle 11| \otimes |I\rangle\rangle\langle\langle U^n|, \tag{4.58}$$

and the condition for the off-diagonal term is given by

$$(\langle\langle (U^*)^n|)|K_0\rangle\rangle = |I\rangle\rangle, \tag{4.59}$$

or equivalently,

$$\lambda|\langle\langle I|(U^{\otimes n} \otimes I_{\mathcal{K}})(|\psi\rangle \otimes |\phi\rangle)| = 1 \tag{4.60}$$

Notice that the maximally entangled state can be written as $|I\rangle\rangle = \sum_i |ii\rangle = \sum_i |\psi_i \psi_i^*\rangle$, where $\{|\psi_i\rangle\}$ is an arbitrary basis, the off-diagonal coherence term can be evaluated as

$$\lambda\langle\langle I|(U^{\otimes n} \otimes I_{\mathcal{K}})(|\psi\rangle \otimes |\phi\rangle) = \lambda\langle\phi^*|(U^{\otimes n})|\psi\rangle \tag{4.61}$$

and its absolute value is $|\lambda||\langle\phi^*|(U^{\otimes n})|\psi\rangle|$. This can achieve 1 only if $|\lambda| = 1$ and $|\psi\rangle = e^{i\theta_U}U^{\otimes n}|\phi\rangle$. Thus, we obtain the necessary condition that $|\psi\rangle$ is invariant under the action of $U^{\otimes n}$. This condition is equivalent to the existence of a one-dimensional invariant subspace of $U^{\otimes n}$, which, by considering the Schur-Weyl duality, happens if and only if n is a multiple of $d = \dim U$. Thus, the necessary condition for most (and fully) coherently controlled unitary operation given by Eq. (4.58) to be implementable, i.e., n is a multiple of d, is derived. This condition is also the sufficient condition, because the quantum circuit shown in Fig. 2.4 of Sec. 2.4.3 implements the controlled unitary operation.

For completeness, the Choi operator for the most coherently controlled neutralization comb is given by

$$\begin{aligned} C_N &= |00\rangle\langle 00| \otimes N + |11\rangle\langle 11| \otimes |I\rangle\rangle\langle\langle I| \\ &\quad + |00\rangle\langle 11| \otimes |K_0\rangle\rangle\langle\langle I| + |11\rangle\langle 00| \otimes |I\rangle\rangle\langle\langle K_0|, \end{aligned} \tag{4.62}$$

$$|S_0\rangle\rangle = |I\rangle\rangle_{0,2N+1} \otimes |A_d\rangle_{\mathcal{H}_{in}} \otimes |A_d\rangle_{\mathcal{H}_{out}}. \tag{4.63}$$

Here $|A_d\rangle$ is the d-dimensional totally antisymmetric state satisfying $U^{\otimes d}|A_d\rangle = (\det U)|A_d\rangle$ for all $U \in U(d)$ given by

$$|A_d\rangle = \frac{1}{\sqrt{d!}} \sum_{\sigma \in \mathcal{S}_d} \mathrm{sgn}(\sigma)|\sigma(1)\rangle|\sigma(2)\rangle \cdots |\sigma(d)\rangle, \tag{4.64}$$

where $\mathcal{S}_d$ is the d-dimensional symmetric group and σ denotes a permutation.

Remark that in this section, we assume that the Choi operator of the neutralization comb has the form of Eq. (4.56), which is implemented by first preparing a quantum state on the auxiliary system, and discard the auxiliary system at the end. If we further restrict the initial state of the auxiliary state to be a pure state, the necessity of the requirement for the initial auxiliary state to be a one-dimensional invariant state is trivial since it is equivalent to an invariant pure state. However, if preparing a mixed state for the initial state of the auxiliary system is allowed, the maximally mixed state, I/d, is invariant under the action of unitary operations. Although the invariant states exist both in the pure and the mixed states, only the pure invariant state can contribute to exactly implementing the fully coherently controlled unitary operation. However, in approximate cases, the maximally mixed state has been utilized for implementing controlled divisible unitary operation with a randomization algorithm shown in Ref. [20] (Fig. 2.3 of Sec. 2.4.3).

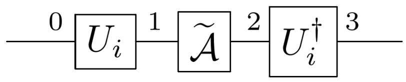


Figure 4.8: Quantum circuit for the basis randomization comb. The input quantum operation is $\widetilde{\mathcal{A}}$, and the action of the basis randomization comb is given by applying a pair of unitary operations, U_i randomly chosen from a set $\{U_i\}$ and its inverse $U_i^\dagger$, before and after the quantum operation $\widetilde{\mathcal{A}}$.

4.4.2 Basis Randomization Comb with the Pauli Operators

In this section and the next section, we consider an approximate neutralization comb employing random unitary operators, which we call a basis randomization comb. The idea of employing random unitary operators to implement controllization of a unitary operation described by Hamiltonian dynamics was introduced in Ref. [20], where randomization is applied to an auxiliary system of which initial state is prepared in the maximally mixed state (see also Sec. 2.4.3 and Fig. 2.3). Here we show that a similar effect can be implemented by applying randomization to the target system directly instead of using an auxiliary system. We consider the two-dimensional case $d = 2$ for simplicity.

While the introduction of a basis randomization comb is intended to apply to infinitesimal Hamiltonian dynamics, i.e., a unitary operation close to the identity operation for obtaining the approximate controllization of Hamiltonian dynamics, the definition of a basis randomization comb is valid for any quantum operation. A generalization of the basis randomization comb for general d-dimensional systems is also straightforward.

Consider a quantum operation $\widetilde{\mathcal{A}} : \mathcal{L}(\mathcal{H}_1 = \mathbb{C}^2) \to \mathcal{L}(\mathcal{H}_2 = \mathbb{C}^2)$ of which Choi operator is given by

$$J_{\mathcal{A}} = \sum_{i,j=0}^{3} c_{ij} |\sigma_i\rangle\!\rangle\langle\!\langle \sigma_j|, \tag{4.65}$$

where $\{\sigma_i\}_{i=0}^3$ represents the set of the Pauli operators and $\{c_{ij}\}_{ij}$ are coefficients. We consider the basis randomization comb $\widetilde{\widetilde{\mathcal{R}}}_S$ implemented by the quantum circuit shown in Fig. 4.8 for a set of unitary operators $S := \{U_i\}$. The unitary operators composing the set S are not necessary to be mutually orthogonal in general. We assume a unitary operator in the set is chosen uniformly randomly with probability $1/|S|$ for simplicity. We analyze the cases for two sets for S, a set consists of the Pauli operators in this section and another set consists of the Clifford operators in Sec. 4.4.3. The action of $\widetilde{\widetilde{\mathcal{R}}}_S$ on $\widetilde{\mathcal{A}}$ denoted as $\langle\widetilde{\mathcal{A}}\rangle_S$ is given by

$$\langle\widetilde{\mathcal{A}}\rangle_S = \frac{1}{|S|}\sum_{U_i\in S}\widetilde{\mathcal{U}}_i^\dagger \circ \widetilde{\mathcal{A}} \circ \widetilde{\mathcal{U}}_i, \tag{4.66}$$

which is implemented by applying a pair of unitary operations, U_i randomly chosen from a set $\{U_i\}$ and its inverse $U_i^\dagger$, before and after the quantum operation $\widetilde{\mathcal{A}}$. The Choi operator of the basis randomization comb $\widetilde{\widetilde{\mathcal{R}}}_S$ is given by

$$R_S = \frac{1}{|S|}\sum_{U_i\in S}|U_i\rangle\!\rangle\langle\!\langle U_i|_{01}\otimes|U_i^\dagger\rangle\!\rangle\langle\!\langle U_i^\dagger|_{23}. \tag{4.67}$$

The Choi operator of the quantum operation transformed by the basis randomization comb $\widetilde{\widetilde{\mathcal{R}}}_S$ for the input quantum operation $\widetilde{\mathcal{A}}$ is given by

$$J_{\langle\mathcal{A}\rangle_S} = \sum_{U_i\in S}\sum_{jk} c_{jk}|U_i^\dagger\sigma_j U_i\rangle\!\rangle\langle\!\langle U_i^\dagger\sigma_k U_i|. \tag{4.68}$$

We investigate the action of the basis randomization comb with a set of the Pauli operators $S_P := \{\sigma_i\}_{i=0}^3$ in this section. A set of the Pauli operators S_P forms a 1-design [59,60]. In the next section, we analyze the basis randomization comb with a set of the Clifford operators S_C, which forms a 1-, 2- and 3- design [59,60] to investigate the difference caused by the sets of unitary operators used in the basis randomization comb.

By using the commutation relation of the Pauli operators, the Choi operator of the resulting quantum operation $J_{\langle\mathcal{A}\rangle_{S_P}}$ is calculated as

$$J_{\langle\mathcal{A}\rangle_{S_P}} = \sum_i c_{ii}|\sigma_i\rangle\!\rangle\langle\!\langle\sigma_i|. \tag{4.69}$$

Thus, the basis randomization comb with S_P transforms the quantum operation $\widetilde{\mathcal{A}}$ to the quantum operation $\langle\mathcal{A}\rangle_{S_P}$ of which Choi operator is given by

$$J_{\langle\mathcal{A}\rangle_{S_P}} = c_{00}\cdot J_{id} + c_{11}\cdot J_X + c_{22}\cdot J_Y + c_{33}\cdot J_Z. \tag{4.70}$$

We first consider a class of unitary operations given by infinitesimal Hamiltonian dynamics of a time-independent Hamiltonian H as $\delta U = e^{-iH\delta t}$. For a unitary operation $\delta\mathcal{U}$ described by a unitary operator $\delta U = e^{-iH\delta t} = I - iH\delta t + O(\delta t^2)$, the Choi operator of the resulting operation by the basis randomization comb $C_{R_{S_P}}$ is calculated as

$$\begin{aligned} J_{\langle\delta U\rangle_{S_P}} = {} & |I\rangle\!\rangle\langle\!\langle I| + \sum_i(-i\sigma_i^\dagger H\sigma_i\delta t)|I\rangle\!\rangle\langle\!\langle I| \\ & + \sum_i |I\rangle\!\rangle\langle\!\langle I|(-i\sigma_i^\dagger H\sigma_i\delta t)^\dagger + O(\delta t^2). \end{aligned} \tag{4.71}$$

We see that the approximate neutralization for any unitary operation in this class with an error of $O(\delta t^2)$ is realized if the second and third terms in Eq. (4.71) vanish.

We further consider a quantum operation given by $U = e^{-iHt}$, and apply the basis randomization comb with S_P for each time interval $\delta t = t/n$ where n is the number of division of the Hamiltonian dynamics in the duration time t. In this case, by considering $\delta U = I - iH\delta t - H^2\delta t^2/2 + O(\delta t^3)$ as the unitary operator for each time interval, we obtain $J_{\langle \delta \mathcal{U} \rangle_{S_P}}$ with coefficients defined by Eq. (4.70) as

$$\begin{aligned} c_{00} &= 1 + [(\mathrm{Tr}H)^2 - d(\mathrm{Tr}H^2)]\delta t^2/d^2 + O(\delta t^4) \\ c_{11} &= (\mathrm{Tr}HX)^2\delta t^2/d^2 + O(\delta t^4) \\ c_{22} &= (\mathrm{Tr}HY)^2\delta t^2/d^2 + O(\delta t^4) \\ c_{33} &= (\mathrm{Tr}HZ)^2\delta t^2/d^2 + O(\delta t^4). \end{aligned} \tag{4.72}$$

When the basis randomization comb is applied n times, the resulting quantum operation is given by $(\langle \delta U \rangle_{S_P})^n$. Since any multiplication of Pauli operations results also a Pauli operation, the Choi operator of this operation can be decomposed in the form of Eq. (4.70), namely,

$$c_0^{(P)} J_{id} + c_1^{(P)} J_X + c_2^{(P)} J_Y + c_3^{(P)} J_Z. \tag{4.73}$$

with the coefficients

$$\begin{aligned} c_0^{(P)} &= 1 + \frac{1}{n}[(\mathrm{Tr}H)^2 - d(\mathrm{Tr}H^2)]\frac{t^2}{d^2} \\ &\quad + \frac{1}{2n^2}\{[(\mathrm{Tr}H)^2 - d(\mathrm{Tr}H^2)]^2 + (\mathrm{Tr}HX)^4 + (\mathrm{Tr}HY)^4 + (\mathrm{Tr}HY)^4]\}\frac{t^4}{d^4} \\ &\quad + O(\frac{1}{n^3}) \end{aligned} \tag{4.74}$$

$$c_1^{(P)} = \frac{1}{n}(\mathrm{Tr}HX)^2\frac{t^2}{d^2} + O(\frac{1}{n^2}) \tag{4.75}$$

$$c_2^{(P)} = \frac{1}{n}(\mathrm{Tr}HY)^2\frac{t^2}{d^2} + O(\frac{1}{n^2}) \tag{4.76}$$

$$c_3^{(P)} = \frac{1}{n}(\mathrm{Tr}HZ)^2\frac{t^2}{d^2} + O(\frac{1}{n^2}). \tag{4.77}$$

Thus, for large enough n, the basis randomization comb with S_P transforms any unitary operation generated by Hamiltonian dynamics to

$$\widetilde{id} + O(1/n), \tag{4.78}$$

which is close to the identity operation, and thus this basis randomization comb is an approximate neutralization comb if it is applied to a unitary operation generated by Hamiltonian dynamics with a small enough interval t/n n times.

The controlled version of (a single element of) this basis randomization comb $C_{R_{S_P}}$ is given by an operator K_0 as

$$C_{R_{S_P}} = |00\rangle\langle 00| \otimes R_{S_P} + |11\rangle\langle 11| \otimes |I\rangle\rangle\langle\langle I| + |00\rangle\langle 11| \otimes |K_0\rangle\rangle\langle\langle I| + |11\rangle\langle 00| \otimes |I\rangle\rangle\langle\langle K_0|. \quad (4.79)$$

Note that the corresponding Kraus representation is given by $\{\frac{1}{2}\sigma_i \otimes \sigma_i^\dagger\}$, and K_0 is in the form of $K_0 = \frac{1}{2}\sum_i \alpha_i^* \sigma_i \otimes \sigma_i^\dagger$ with $\sum_i |\alpha_i|^2 = 1$. The action of R_{S_P} on the Choi operator of an arbitrary unitary operation $|U\rangle\rangle\langle\langle U|$ is

$$\mathrm{Tr}_{12}[R_{S_P}(|U\rangle\rangle\langle\langle U|)^T] = |00\rangle\langle 00| \otimes J_{\langle U\rangle_{S_P}} + |11\rangle\langle 11| \otimes J_U + |11\rangle\langle 00| \otimes \langle\langle U^*||I\rangle\rangle\langle\langle K_0||U^*\rangle\rangle + h.c., \quad (4.80)$$

and $\langle\langle U^*||K_0\rangle\rangle$ in the off-diagonal coherence term is evaluated as

$$\begin{aligned}\langle\langle U^*||K_0\rangle\rangle &= \langle\langle I|_{12}(I_1 \otimes U_2^T) \cdot \frac{1}{2}(\sum_i \alpha_i^*(\sigma_i)_1 \otimes (\sigma_i^*)_2)(|I\rangle\rangle_{01} \otimes |I\rangle\rangle_{23}) \\ &= \frac{1}{2}\langle\langle I|(\sum_i \alpha_i^*(\sigma_i^\dagger U \sigma_i)_1 \otimes I_2)(|I\rangle\rangle_{01} \otimes |I\rangle\rangle_{23}) \\ &= \frac{1}{2}|\sum_i \alpha_i^*(\sigma_i^\dagger U \sigma_i)\rangle\rangle_{03}, \end{aligned} \quad (4.81)$$

where the subscripts denote the indices of the Hilbert spaces of the target system.

By requiring the most coherently controlled identity operation on the target system to be the identity operation in the extended system including the control system, i.e., $I \mapsto |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes I$, Eq. (4.81) should satisfy

$$\begin{aligned}\frac{1}{2}|\sum_i \alpha_i^*(\sigma_i^\dagger I \sigma_i)\rangle\rangle_{03} &= |I\rangle\rangle_{03}, \\ \sum_i \alpha_i &= 2. \end{aligned} \quad (4.82)$$

Thus, the coefficients are $\alpha_i = 1/2$ for all i, and the operator K_0 is uniquely determined as

$$K_0 = \frac{1}{4}(I \otimes I + X \otimes X + Y \otimes Y + Z \otimes Z), \quad (4.83)$$

and we obtain

$$\langle\langle U^*||K_0\rangle\rangle = \frac{1}{4}|\sum_i(\sigma_i^\dagger U \sigma_i)\rangle\rangle_{03}. \quad (4.84)$$

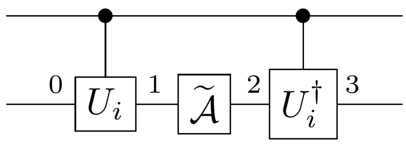


Figure 4.9: A quantum circuit for the controlled basis randomization comb. The input quantum operation is $\widetilde{\mathcal{A}}$, and the action of the basis randomization comb is given by applying a pair of controlled unitary operations C_{U_i} chosen uniform randomly from a set $\{U_i\}$ and its inverse $C_{U_i}^\dagger$ before and after the quantum operation $\widetilde{\mathcal{A}}$. By repeating this circuit n times, the controlled unitary operation of Hamiltonian dynamics $U = e^{-iHt}$ is implemented with an error of $O(1/n)$ with the global phase factor $\theta_U = (\mathrm{Tr}H/d)t$.

A Kraus representation of this most coherently controlled neutralization comb is given by

$$\begin{aligned}\{&|0\rangle\langle 0| \otimes I \otimes I + |1\rangle\langle 1| \otimes I \otimes I,\\ &|0\rangle\langle 0| \otimes X \otimes X + |1\rangle\langle 1| \otimes I \otimes I,\\ &|0\rangle\langle 0| \otimes Y \otimes Y + |1\rangle\langle 1| \otimes I \otimes I,\\ &|0\rangle\langle 0| \otimes Z \otimes Z + |1\rangle\langle 1| \otimes I \otimes I\},\end{aligned} \tag{4.85}$$

and one possible implementation in the quantum circuit is shown in Fig. 4.9.

When we apply the controlled basis randomization comb n times, since this comb does not change the state of the control qubit, the term corresponding to Eq. (4.81) is evaluated as

$$I \otimes \frac{1}{4^n}(\sum_i \sigma_i^\dagger U \sigma_i)^n |I\rangle\rangle. \tag{4.86}$$

For the case $U = e^{-iH\delta t} = I - iH\delta t - H^2\delta t^2/2 + O(\delta t^3)$ with $\delta t = t/n$, we have

$$\begin{aligned}\frac{1}{4}(\sum_i \sigma_i^\dagger U \sigma_i) &= I - i\delta t(\frac{1}{4}\sum_i \sigma_i^\dagger H \sigma_i) - \frac{1}{2}\delta t^2(\frac{1}{4}\sum_i \sigma_i^\dagger H^2 \sigma_i) + O(\delta t^3)\\ &= I - i\delta t(\mathrm{Tr}H)I/d - \frac{1}{2}\delta t^2(\mathrm{Tr}H^2)I/d + O(\delta t^3),\end{aligned} \tag{4.87}$$

and we obtain

$$\frac{1}{4^n}(\sum_i \sigma_i^\dagger U \sigma_i)^n = e^{-i(\mathrm{Tr}H/d)t} I + O(1/n). \tag{4.88}$$

Finally, we obtain the Choi operator of the quantum operation transformed from $U = e^{-iHt}$ by the controlled basis randomization comb with S_P as

$$|00\rangle\langle 00| \otimes J_{id} + |11\rangle\langle 11| \otimes J_U + |11\rangle\langle 00| \otimes |e^{i(\mathrm{Tr}H/d)t}U\rangle\rangle\langle\langle I| + h.c. + O(1/n), \tag{4.89}$$

which converges to the (fully coherently) controlled unitary operation, that is $C_{e^{-iHt}} = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes e^{i(\mathrm{Tr}H/d)t}e^{-iHt}$ in the limit of $n \to \infty$.

4.4.3 Basis Randomization Comb with the Clifford Operators

In the previous section, we considered the basis randomization using a set of the Pauli operators S_P, for erasing the terms of $O(\delta t)$ in Eq. (4.71). The Choi operator of the resulting operation by the basis randomization comb given by Eq. (4.68) is of the form $\sum_i (U_i^\dagger \otimes U_i^T) J_{\mathcal{A}} (U_i^\dagger \otimes U_i^T)^\dagger$. Since the Choi operator of the identity operation, $|I\rangle\rangle\langle\langle I|$, is the fixed point of $\int dU (U^\dagger \otimes U^T) \cdot (U^\dagger \otimes U^T)^\dagger$, it is expected that this integral transforms any Choi operator approximately to $|I\rangle\rangle\langle\langle I|$.

The corresponding effect can be achieved for $\sum_i (U_i^\dagger \otimes U_i^T) \cdot (U_i^\dagger \otimes U_i^T)^\dagger$ if we choose the set $S = \{U_i\}$ to be a 2-design (by definition of 2-design) [60]. Thus, the basis randomization by a 2-design may perform better than a 1-design, that is, the Pauli operators. In this section, we analyze the basis randomization comb employing a 2-design using a set of the Clifford operators of a 1-qubit system.

We first summarize the properties of the Clifford group that we use in the following [61]. Clifford group G_C is the group of the operators by whom conjugation transforms any Pauli operator into another Pauli operator, that is,

$$\forall U \in S_P,\ \forall V \in G_C,\ VUV^\dagger \in S_P. \tag{4.90}$$

Note that the Clifford group has a trivial center Z

$$Z = \{\pm I, \pm iI, \pm e^{i\frac{\pi}{4}} I, \pm e^{3i\frac{\pi}{4}} I\}, \tag{4.91}$$

of which element can only change the global phase, and thus, we only consider R_C, the residue class of G_C divided by Z as $R_C := G_C/Z$. Since the set of the Pauli operators S_P is a normal subgroup of R_C, we can define the residue group $R_{C/P} := R_C/S_P$.

The representative elements of $R_{C/P}$ are given by the following six operators

$R_{C/P} = \{V_\sigma\}$, where σ denotes a permutation among $\{1, 2, 3\}$,

$$V_{\mathrm{id}} = I \tag{4.92}$$

$$V_{(1,2)} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \tag{4.93}$$

$$V_{(2,3)} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\frac{\pi}{4}} & e^{-i\frac{\pi}{4}} \\ e^{-i\frac{\pi}{4}} & e^{i\frac{\pi}{4}} \end{pmatrix} \tag{4.94}$$

$$V_{(3,1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{4.95}$$

$$V_{(1,2,3)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \tag{4.96}$$

$$V_{(3,2,1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}. \tag{4.97}$$

The Choi operator $J_{\langle\mathcal{A}\rangle_{R_C}}$ of the quantum operation $\widetilde{\mathcal{A}}$ transformed by the basis randomization comb with the set of the Clifford operators R_C is given by

$$J_{\langle\mathcal{A}\rangle_{R_C}} = \frac{1}{24} \sum_{k,l=0}^{3} \sum_{\sigma_i \in S_P} \sum_{V_j \in R_{C/P}} c_{kl} |\sigma_i^\dagger V_j^\dagger \sigma_k V_j \sigma_i\rangle\!\rangle\langle\!\langle \sigma_i^\dagger V_j^\dagger \sigma_l V_j \sigma_i|. \tag{4.98}$$

Since $V_j^\dagger \sigma_k V_j$ and $V_j^\dagger \sigma_l V_j$ are Pauli operators by definition of the Clifford operators, we obtain

$$J_{\langle\mathcal{A}\rangle_{R_C}} = \frac{1}{6} \sum_{i=0}^{3} \sum_{V_j \in R_{C/P}} c_{ii} |V_j^\dagger \sigma_i V_j\rangle\!\rangle\langle\!\langle V_j^\dagger \sigma_i V_j|. \tag{4.99}$$

By using the following equation for the Pauli operators $U_i (= \sigma_i)$ with $i = 0, 1, 2, 3$,

$$|V_\sigma U_i V_\sigma^\dagger\rangle\!\rangle\langle\!\langle V_\sigma U_i V_\sigma^\dagger| = |U_{\sigma(i)}\rangle\!\rangle\langle\!\langle U_{\sigma(i)}|, \tag{4.100}$$

where we set $\sigma(0) = 0$, we obtain

$$J_{\langle\mathcal{A}\rangle_{R_C}} = c_{00} \cdot J_{id} + \frac{c_{11} + c_{22} + c_{33}}{3} (J_X + J_Y + J_Z). \tag{4.101}$$

With the depolarizing channel $\widetilde{\mathcal{D}}$, the Choi operator of the resulting operation is also represented as

$$J_{\langle\mathcal{A}\rangle_{R_C}} = \left(c_{00} - \frac{c_{11} + c_{22} + c_{33}}{3} \right) J_{id} + \frac{4}{3} (c_{11} + c_{22} + c_{33}) J_{\mathcal{D}}. \tag{4.102}$$

Similar to the case of the basis randomization comb with S_P, we consider the quantum operation given by a time-independent Hamiltonian H, i.e., $U = e^{-iHt}$, and apply the basis randomization comb for each time interval $\delta t = t/n$. When the basis randomization with R_C is applied n times, the Choi operator of the resulting operation is given by

$$c_0^{(C)} J_{id} + c_1^{(C)} J_X + c_2^{(C)} J_Y + c_3^{(C)} J_Z. \tag{4.103}$$

with the coefficients

$$\begin{aligned} c_0^{(C)} &= 1 + \frac{1}{n}[(\mathrm{Tr}H)^2 - d(\mathrm{Tr}H^2)]\frac{t^2}{d^2} \\ &+ \frac{1}{2n^2}\{[(\mathrm{Tr}H)^2 - d(\mathrm{Tr}H^2)]^2 + \frac{1}{3}[(\mathrm{Tr}HX)^2 + (\mathrm{Tr}HY)^2 + (\mathrm{Tr}HY)^2]^2\}\frac{t^4}{d^4} \\ &+ O(\frac{1}{n^3}) \end{aligned} \tag{4.104}$$

$$c_1^{(C)} = c_2^{(C)} = c_3^{(C)} = \frac{1}{3n}[(\mathrm{Tr}HX)^2 + (\mathrm{Tr}HY)^2 + (\mathrm{Tr}HY)^2]\frac{t^2}{d^2} + O(\frac{1}{n^2}). \tag{4.105}$$

The coefficient of J_{id} coincides with that for the case with S_P up to the order $1/n$. However, the basis randomization comb with R_C performs worse than the case with S_P in the sense that the coefficient of J_{id} is smaller, when the terms of $O(1/n^2)$ are considered. The basis randomization comb with R_C transforms any unitary operation generated by Hamiltonian dynamics to

$$\widetilde{id} + O(1/n), \tag{4.106}$$

which is close to the identity operation with an error of $O(1/n)$, and thus this basis randomization comb is an approximate neutralization comb.

The most coherently controlled version of (a single element of) the basis randomization comb $C_{R_{R_C}}$ is determined by an operator K_0 similar to the case of S_P. The Kraus representation of the basis randomization comb with R_C is given by $\{\frac{1}{\sqrt{24}} U_i \otimes U_i^\dagger \mid U_i \in R_C\}$. Since the dimension of the linear span of $\mathcal{L}(\mathbb{C}^2 \otimes \mathbb{C}^2)$ is 16 while this set contains 24(> 16) elements, this set of operators is over-complete. Thus, it is necessary to derive another Kraus representation with a set of orthogonal Kraus operators for proceeding our analysis. The span of the Kraus operators is invariant under the swap operation U_{swap} between the first and the second Hilbert space, because any element is of the form $K = \sum_i \alpha_i U_i \otimes U_i^\dagger$ with $U_i \in R_C$, and $U_{swap} K U_{swap}$ is also in the span. Thus, the span is in the $d(d+1)/2 = 10$ dimensional symmetric subspace. By calculating the spectral decomposition of the Choi operator corresponding to this Kraus representation, we can check that the Kraus operators actually span the 10-dimensional symmetric subspace. Specifically, the Kraus operators are given by

$$\{K_0 = \frac{1}{4}(I\otimes I + X\otimes X + Y\otimes Y + Z\otimes Z), K_1, \dots, K_9\}, \tag{4.107}$$

where $\{K_i\}$ is a set of orthogonal operators in the symmetric subspace satisfying $\mathrm{Tr}K_i^\dagger K_i = 1/3$ for $i = 1, \dots, 9$. Note that $\mathrm{Tr}K_0^\dagger K_0 = 1$. Thus, the off-diagonal coherent term of the most coherent controlled comb is characterized by

$$K_0 = \frac{1}{4}(I\otimes I + X\otimes X + Y\otimes Y + Z\otimes Z), \tag{4.108}$$

which coincides to the case with the basis randomization with the Pauli operators[2]. This indicates that the maximum off-diagonal coherent term is the same for controllization of the basis randomization comb with S_P and R_C for up to $O(1/n)$ approximation.

Since the basis randomization comb with R_C does not behave better than the one with S_P for Hamiltonian dynamics with the terms of up to $O(1/n)$, and the coherent terms of both cases coincide, we conclude that using the Clifford operators for randomization does not improve controllization of Hamiltonian dynamics. Moreover, the analysis of the terms with $O(1/n^2)$ shows that the performance of the basis randomization with R_C as approximate neutralization turns out to be worse than that of S_P in general. That is, the difference of the coefficients given by Eq. (4.74) and Eq. (4.104) satisfies

$$c_0^{(P)} - c_0^{(C)} = \frac{1}{2n^2}(d_1^2 + d_2^2 + d_3^2) \geq 0, \tag{4.109}$$

where

$$d_1 = \frac{1}{3}[2(\mathrm{Tr}HX)^2 - (\mathrm{Tr}HY)^2 - (\mathrm{Tr}HZ)^2]\frac{t^2}{d^2} \tag{4.110}$$

$$d_2 = \frac{1}{3}[2(\mathrm{Tr}HY)^2 - (\mathrm{Tr}HX)^2 - (\mathrm{Tr}HZ)^2]\frac{t^2}{d^2} \tag{4.111}$$

$$d_3 = \frac{1}{3}[2(\mathrm{Tr}HZ)^2 - (\mathrm{Tr}HX)^2 - (\mathrm{Tr}HY)^2]\frac{t^2}{d^2}. \tag{4.112}$$

This difference can be understood by rewriting Eq. (4.70) as

$$\begin{aligned} J_{\langle\mathcal{A}\rangle_{S_P}} =& \left(c_{00} - \frac{c_{11}+c_{22}+c_{33}}{3}\right) J_{id} + \frac{4}{3}\left(c_{11}+c_{22}+c_{33}\right) J_{\mathcal{D}} \\ &+ \frac{1}{3}(2c_{11} - c_{22} - c_{33})J_X + \frac{1}{3}(2c_{22} - c_{11} - c_{33})J_Y + \frac{1}{3}(2c_{33} - c_{11} - c_{22})J_Z. \end{aligned} \tag{4.113}$$

[2]Precisely, the global phase is not uniquely determined by maximizing the Hilbert-Schmidt norm of the operator, and $e^{i\theta}K_0$ for any real parameter θ is also a candidate instead of K_0. We choose $\theta = 0$ by requiring the most coherently controlled version of the identity operation to be also the identity operation, i.e., $I \mapsto |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes I$.

Compared to Eq. (4.102), there are extra terms of Pauli operations which contributes to the coefficient of the identity operation, as the identity operation can be obtained by applying the same Pauli operation twice. In conclusion, it is enough to use S_P for the task of controllization of Hamiltonian dynamics using the most coherently controlled basis randomization comb.

4.5 Conclusion

We have defined a controlled quantum operation of a general deterministic quantum operation based on two physical implementations and a set of axioms, which coincide with each other. We then analyzed the coherence between the quantum operations on different control qubit states, and gave a characterization of the controlled quantum operations that maximize the coherence, which we call the most coherently controlled quantum operation. This definition of controlled quantum operation is extended to quantum combs, and we defined controlled quantum combs and the most coherently controlled quantum combs.

We investigated a relationship between quantum switch and controlled quantum operations with our definition. We also showed a relation between controlled quantum operations and controlled quantum combs, by introducing the neutralization combs. We presented a method to analyze controllization, and provided a new algorithm for approximate controllization of divisible unitary operations using the basis randomization combs. We also evaluated the performance of the basis randomization combs employing the Pauli operators and the Clifford operators, and showed that the randomization by the Pauli operators performs better in this controllization algorithm.

Chapter 5

Success-or-Draw Implementation of Probabilistic Higher-order Quantum Operations

Implementing higher-order quantum operations within quantum mechanics is not straightforward and often impossible, especially in an exact and deterministic manner. In order to implement higher-order quantum operations, two types of relaxations are usually considered: approximate implementation and probabilistic implementation. The approximate implementation of higher-order quantum operations has an advantage, as such an implementation is always available by utilizing quantum process tomography [40]. However, the figure of merit, usually evaluated by the average fidelity F, for the method based on quantum process tomography is expected to scale as $1-1/poly(N)$ given N uses of the input operation. The probabilistic implementation, on the other hand, can achieve a success probability converges to one exponentially, if it is possible to perform a repeat-until-success strategy, namely, perform independent trials until succeed. However, such a strategy requires the initial resource, the input quantum operations and the input quantum state, to be prepared for every trial. In quantum mechanics, cloning of the unknown input state is forbidden by the no-cloning theorem [7], and transformations usually disturb the input state [4, 62] regardless of success or failure. Thus, performing independent trials for probabilistic higher-order quantum operations is not straightforward in general.

In this chapter, we propose a structure for probabilistic higher-order quantum operations called "*success-or-draw*" (Fig. 5.1a). In a usual probabilistic higher-order quantum operation, the input state is lost when it fails, because an unknown quantum operation is applied to the state in general. We propose a probabilistic higher-order quantum operation which "keeps" the input

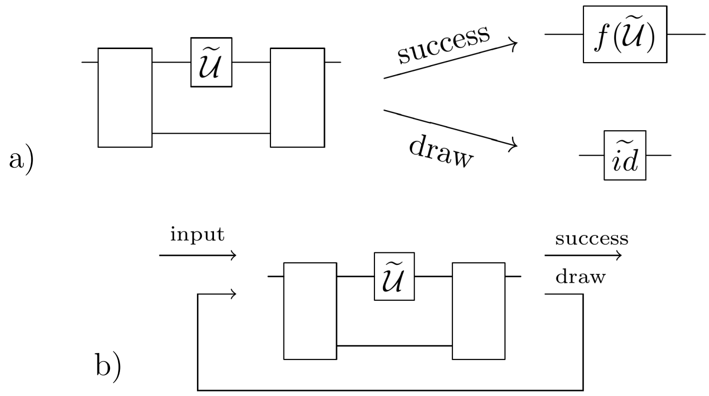


Figure 5.1: Success-or-draw higher-order quantum operations have a structure that the output state remains in the initial state when the higher-order quantum operation fails. Since the initial state is not altered on failure, one can re-iterate this higher-order quantum operation to obtain an exponentially decreasing failure probability. Fig. 5.1a represents the action of a success-or-draw higher-order quantum operation: when it succeeds, the target operation $f(\widetilde{\mathcal{U}})$ is applied; and when it draws, the identity operation $\widetilde{id}$ is applied. Fig. 5.1b illustrates a repeat-until-success strategy which is allowed by the success-or-draw structure.

quantum state on failure, or we call it a *draw* as we are able to perform another trial when it happens as shown in Fig. 5.1b. In Sec. 5.1, we provide a mathematical formulation of the success-or-draw structure. In Sec. 5.2, we show that the success-or-draw structure can be achieved for a large class of higher-order quantum operations. In Sec. 5.3, we analyze unitary inversion with the success-or-draw structure. We show that a better success probability is achievable compared to the previously known value [13] for unitary inversion with two uses of an input unitary operation, and that the success-or-draw structure is not possible for unitary inversion with a single use of an input unitary operation.

5.1 The Success-or-Draw Structure

Consider a probabilistic higher-order quantum operation, especially a probabilistic comb, transforming unitary operations $\{\widetilde{\mathcal{U}}\}$ into CPTP maps $\{f(\widetilde{\mathcal{U}})\}$, where f is a supermap of which output is guaranteed to be a CPTP map for any input unitary operation. In usual settings of a probabilistic higher-order quantum operation, this problem is formulated by the constraints

$$\widetilde{\widetilde{\mathcal{S}}}(\widetilde{\mathcal{U}}) = p_U f(\widetilde{\mathcal{U}}) \tag{5.1}$$

$$S \geq 0, F \geq 0 \tag{5.2}$$

$$S + F \text{ is a deterministic comb,} \tag{5.3}$$

where $\widetilde{\widetilde{\mathcal{S}}}$ and $\widetilde{\widetilde{\mathcal{F}}}$ are the probabilistic combs describing the action of the higher-order quantum operation on success and failure, respectively, and S and F are the corresponding Choi operators.

For the success-or-draw higher-order quantum operation, the action on failure is also determined, and extra constraints on $\widetilde{\widetilde{\mathcal{F}}}$ are required. For the convenience of the following discussions, we also assume that the input unitary operation $\widetilde{\mathcal{U}}$ is used K times. Since any unitary operation must be transformed into the identity operation on failure to guarantee the draw property, the corresponding constraints are given by

$$\widetilde{\widetilde{\mathcal{S}}}(\widetilde{\mathcal{U}}^{\otimes K}) = p_U f(\widetilde{\mathcal{U}}) \tag{5.4}$$

$$\widetilde{\widetilde{\mathcal{N}}}(\widetilde{\mathcal{U}}^{\otimes K}) \propto \widetilde{id} \tag{5.5}$$

$$S \geq 0, N \geq 0 \tag{5.6}$$

$$S + N \text{ is a deterministic comb,} \tag{5.7}$$

where $\widetilde{id}$ denotes the identity operation, indicating that the input state does not change on failure. Here we use $\widetilde{\widetilde{\mathcal{N}}}$ instead of $\widetilde{\widetilde{\mathcal{F}}}$ to denote that it corresponds to draw instead of failure.

5.2 Universal Construction of Success-or-Draw on Unitary Operations

Theorem 5.1 presents the realizability of success-or-draw higher-order quantum operation. A pictorial interpretation of Theorem 5.1 is given by Fig. 5.2.

Theorem 5.1. *Given a probabilistic comb transforming d-dimensional unitary operations $\{\widetilde{\mathcal{U}}\}$ to CPTP maps $\{f(\widetilde{\mathcal{U}})\}$ as $\widetilde{\widetilde{\mathcal{S}}}_t : \widetilde{\mathcal{U}} \mapsto p_U f(\widetilde{\mathcal{U}})$. Then there exist $\varepsilon > 0$ and a set of probabilistic combs $\widetilde{\widetilde{\mathcal{S}}}$ and $\widetilde{\widetilde{\mathcal{N}}}$ summing up to a deterministic comb, which actions are given by*

$$\widetilde{\widetilde{\mathcal{S}}} : \widetilde{\mathcal{U}}^{\otimes d} \mapsto \varepsilon p_U f(\widetilde{\mathcal{U}}) \tag{5.8}$$

$$\widetilde{\widetilde{\mathcal{N}}} : \widetilde{\mathcal{U}}^{\otimes d} \mapsto (1 - \varepsilon p_U)\widetilde{id}. \tag{5.9}$$

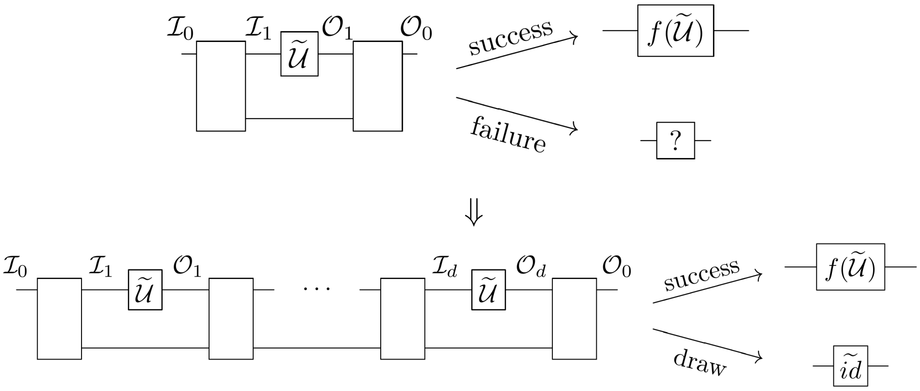


Figure 5.2: A pictorial interpretation of Theorem 5.1. We consider the case when there exists a probabilistic comb (upper) that transforms a unitary operation $\widetilde{\mathcal{U}}$ into a CPTP map $f(\widetilde{\mathcal{U}})$ for all d-dimensional unitary operations $\widetilde{\mathcal{U}}$, and its action is arbitrary on failure. Theorem 5.1 states that in this case, there exists a d-slot probabilistic comb (lower) that performs the same action on success, and performs the identity operation on failure/draw, which corresponds to the preservation of the input state.

The details of the proof is given in Appendix C. In order to prove Theorem 5.1, we first prove Lemma C.1 and Lemma C.2, which indicate that it is enough to prove another theorem presented in the Applendix C, Theorem C.1. Here we state the sketch of the proof.

Sketch of the proof. The proof is constructive. We present a construction of S and N, the Choi operators of $\widetilde{\widetilde{\mathcal{S}}}$ and $\widetilde{\widetilde{\mathcal{N}}}$, from S_t, the Choi operator of $\widetilde{\widetilde{\mathcal{S}}}_t$. The requirements for the combs are given by Eqs. (5.4)-(5.7), which need to be satisfied simultaneously.

Lemma C.1 provides a sufficient condition of the neutralization condition Eq. (5.5). The neutralization condition Eq. (5.5) is difficult to utilize for many reasons, for example, the probability for neutralization is not constant in general. In Theorem 5.1, the probability of neutralization can depend on U. A direct way to rewrite Eq. (5.5) is to add new variables $\{q_U\}$ that corresponds to the probability depend on U and rewrite as

$$\widetilde{\widetilde{\mathcal{N}}}(\widetilde{\mathcal{U}}^{\otimes K}) = q_U \cdot \widetilde{id}. \tag{5.10}$$

Since the corresponding Choi operators are positive, and that for r.h.s. is a rank-1 operator, this condition can be reduced to an inequality of the form

$$\widetilde{\widetilde{\mathcal{N}}}(\widetilde{\mathcal{U}}^{\otimes K}) \leq c \cdot \widetilde{id}, \tag{5.11}$$

where c is a constant determined by the normalization conditions. This condition is equivalent to the one given by Eq. (5.5), but it is still difficult to analyze because it is necessary to consider all unitary operations. Note that in numerical analysis, it is possible to use this condition directly as in Sec. 5.3. In Lemma C.1, we provide a sufficient condition by considering a symmetric subspace, that is, $\widetilde{\mathcal{U}}^{\otimes K}$ is invariant under permutations of each input unitary operations.

Lemma C.2 provides a characterization of the Choi operator of a probabilistic comb transforming unitary operations to CPTP maps, which is the assumption of Theorem 5.1. We consider a Hermitian basis which consists of an identity operator and traceless operators, and show that the decomposition of the corresponding Choi operator consists of only certain terms. Using a basis with an identity operator and traceless operators is convenient for considering the causal condition given by Eqs. (2.23)-(2.25), because the traceless terms help in determining which terms do not affect the causal condition.

By considering Lemma C.1 and Lemma C.2, it is enough to prove another theorem, Theorem C.1, in order to prove Theorem 5.1. The proof of Theorem C.1 can be further divided into two parts: the first part presents a construction of the Choi operators S and the partial trace of N given by $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}} = \mathrm{Tr}_{\mathcal{O}_0}N$ from S_t; the second part is mainly separated into Lemma C.4, which presents a construction of N from $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$.

In the first part of the proof, we first present a trivial set of Choi operators S and F from S_t, where F is a Choi operator which does not necessarily satisfy the neutralization condition Eq.(5.5) for N, but satisfies all the remaining conditions given by Eqs. (5.4),(5.6),(5.7). Moreover, F also has a similar decomposition given by Lemma C.2. We then present a construction of $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$ from F, where the neutralization condition is also satisfied in addition to the positivity Eq. (5.6) and the causal conditions Eq. (5.7). The positivity of $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$ is satisfied by taking the operator to be a strictly positive full-rank operator, and the main difficulty is to satisfy the causal condition and the neutralization condition simultaneously. The decomposition given by Lemma C.2 is convenient for the causal condition in the sense that it is possible to add certain traceless terms that do not affect the causal condition, and we give a class of Choi operators that satisfies the causal condition. Then, we show that among this class of Choi operators, it is possible to cancel the terms that do not satisfy the neutralization condition by using the properties of the symmetric subspace considered in Lemma C.1. Thus, it is possible to satisfy the causal condition and the neutralization condition simultaneously.

In the second part of the proof, we construct N from $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$. In this part, the causal condition and the neutralization condition are easily satisfied because the

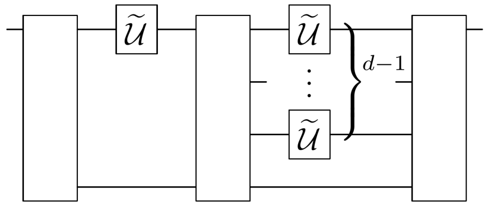


Figure 5.3: The constructed success-or-draw comb in the proof of Theorem C.1 has an extra structure: it uses one copy of the unitary operation at first, and then uses the remaining $d-1$ copies of the unitary operation in parallel.

condition is similar to the first part. On the other hand, the positivity condition becomes difficult. Unlike in the first part, since the target operation is the identity channel of which Choi operator is rank-1, the Choi operator N cannot be a full-rank operator, which is robust in positivity. To solve this problem, we consider a subspace of the Hilbert space that N is on, and we show a construction of N that lies in this subspace and is a strictly positive full-rank operator in the subspace. Thus, the positivity of N can be satisfied. We remark that when the indefinite causal order is considered, the construction of N from $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$ can be replaced by a simpler one by exploiting the symmetry as Remark C.1, and a higher success probability can be achieved in general.

□

While we only require that $S+N$ is a deterministic comb, that is, the input operations are used in a sequential way, the construction shown in the proof of Theorem C.1 (Eq. (C.36)) satisfies an extra condition

$$\mathrm{Tr}_{\mathcal{O}_0}(S+N) = \mathrm{Tr}_{\mathcal{O}_2\mathcal{O}_3\cdots\mathcal{O}_d\mathcal{O}_0}(S+N) \otimes \frac{I_{\mathcal{O}_2\mathcal{O}_3\cdots\mathcal{O}_d}}{d^{d-1}}. \tag{5.12}$$

This condition shows that the comb can be decomposed into two blocks as the quantum circuit shown in Fig. 5.3: the first block uses only a single unitary operation, while the second block uses the remaining $d-1$ unitary operations in parallel. Such a structure indicates that while the number of uses increases with d, the depth of this comb is constant as two. Note that we can assume this structure if we only consider non-zero success probability, and in general, adding this assumption would decrease the success probability.

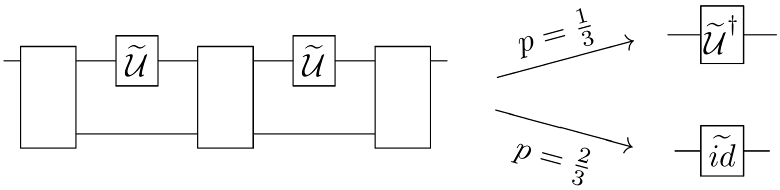


Figure 5.4: The success-or-draw protocol for unitary inversion. When the unitary operation can be used twice, the optimal success probability for success is 1/3, whereas that of the optimal success-or-resetting protocol is 1/4. In either case, the output on failure is the identity operation, which means the initial input state is preserved and it is possible to run the same protocol again with extra uses of the input unitary operation.

5.3 Unitary Inversion with the Success-or-Draw Structure

In this section, we analyze the probabilistic unitary inversion with the success-or-draw structure of a higher-order quantum operation. We only consider the two-dimensional case $d = 2$ in this section. The optimal success probability can be obtained by the following SDP

$$\max \quad p \tag{5.13}$$
$$\text{s.t.} \quad \mathrm{Tr}_{\mathcal{IO}}[S({J_{U_i}}^{\otimes K})^T] = pJ_{U_i^{-1}} \tag{5.14}$$
$$\mathrm{Tr}_{\mathcal{IO}}[N({J_{U_i}}^{\otimes K})^T] \leq d^K J_{id} \tag{5.15}$$
$$S \geq 0, N \geq 0 \tag{5.16}$$
$$S + N \text{ is a deterministic comb,} \tag{5.17}$$

where $\{U_i\}$ is a finite set of unitary operators that the corresponding Choi operators forms a basis of the linear span of $\mathrm{span}\{J_U^{\otimes k}\}$ (see Refs. [13, 14]). Note that Lemma C.1 is not used because it is a sufficient condition and may lower the success probability.

For $K = 2$, Theorem 5.1 indicates that the optimal success probability is positive as $p > 0$. A numerical solution to this SDP shows that the optimal success probability is $p = 1/3$. In Ref. [13] (Sec. 2.6.2), an explicit quantum circuit with the success-or-draw structure is presented which success probability is 1/4. One difference between the optimal success-or-draw protocol we numerically obtained and the protocol presented in Ref. [13] is that the latter is not only a success-or-draw protocol, but it has another feature: it can be regarded as a success-or-resetting protocol. The latter protocol uses a single copy of a unitary operation to obtain its inverse, and when it fails, it results in a state that is "resettable" to be the input state by another unitary operation. While such a success-or-resetting protocol usually has a lower success probability, it has an advantage as we can choose whether to continue the protocol by resetting after we know if it succeeded.

For $K = 1$, we prove that the optimal success probability is $p = 0$, which means it is not possible to have a success-or-draw structure. The proof is given in Appendix D. This result gives an explicit example that a success-or-draw structure is not available.

In Theorem 5.1, we show that it is possible to obtain a success-or-draw protocol with $K = d$ uses of the input unitary operation, and this results shows that $K = d - 1$ uses is not enough for $d = 2$. We conjecture that it is not possible to obtain a success-or-draw protocol with $K = d - 1$ uses of the input unitary operation in Theorem 5.1 for general d. One reason for this conjecture is that in the construction of the success-or-draw protocol in Theorem 5.1, the totally antisymmetric state plays an important role, and such a state only exists in a d qudit system.

5.4 Conclusion

We have introduced a new structure for probabilistic higher-order quantum operations which we name success-or-draw structure. A probabilistic higher-order quantum operation with the success-or-draw structure can amplify its success probability by using multiple copies of the input quantum operation in a sequential manner, which scales exponentially to one in the number of uses. We presented a mathematical formulation for the success-or-draw higher-order quantum operation. We considered the case where the input quantum operation is a unitary operation, and we proved that any probabilistic higher-order quantum operation transforming unitary operations into CPTP maps is compatible with the success-or-draw structure by adding the number of uses of the unitary operation.

We then analyzed the problem of the two-dimensional unitary inversion. When two uses of an input unitary operation are allowed, Theorem 5.1 guarantees the existence of a non-trivial solution to this problem, and we obtained the optimal solution numerically using SDP. A success-or-draw protocol for this problem was also presented previously in Ref. [13], and our numerical calculation shows that a higher success probability can be achieved if we only require the success-or-draw structure. We also proved that a success-or-draw strategy does not exist with a single use of an input unitary operation.

Chapter 6

Conclusion and Future Scope

In this thesis, we considered three topics on higher-order quantum operations: the uniqueness on the definition of quantum switch; a framework for controlled quantum operations and higher-order quantum operations and controllization; and the success-or-draw structure for probabilistic higher-order quantum operations. We provided new methods for the analysis of higher-order quantum operations, which can be used as fundamental building blocks for further theoretical studies of higher-order quantum operations. We also contribute to the experimental realization of higher-order quantum operations by proposing new quantum algorithms for efficient implementations of certain higher-order quantum operations.

In the first topic, we analyzed the uniqueness of the definition of quantum switch, and provided a comprehensive background for the studies on quantum switch. We proved that even if we only define the action of quantum switch on only unitary operations, its action is also uniquely defined on general quantum operations by setting the requirements of the single use and the positivity of the corresponding Choi operator, which is necessary for its physical implementation.

Besides quantum switch, many higher-order quantum operations are only defined for unitary operations such as unitary inversion. In Ref. [17], it is proven that the action of two-dimensional unitary inversion is uniquely extended to general quantum operations under the extra requirements of the single use and the positivity of the corresponding Choi operator. However, it is not known if there exist other higher-order quantum operations of which uniqueness of the extension can be shown except for trivial cases. Quantum switch with more than two input operations is such an example. In the proof for quantum switch with two input operations, we reduced the problem of the uniqueness to a problem of counting. A similar method may be possible even if a greater number of input operations is considered, but the counting may become more difficult. It is not known whether there exist other methods for proving the uniqueness. A general method for proving the uniqueness of a certain function is to consider the difference between a candidate and the target function, and prove the difference vanishes. However, this method does not work well in our case because when the difference is considered, it is not obvious how the positivity condition of the Choi operator can be used.

When multiple uses of an input operation are allowed, the action on unitary operation cannot be uniquely determined for general quantum operations in general. In particular, if a higher-order quantum operation can be implemented with K uses of an input operation, then if more than K uses is allowed, the uniqueness does not hold because it is always possible to discard a certain number of input operations. Even though, if it is possible to restrict the form of supermap using certain assumptions such as the positivity of the Choi operator, the analysis of the performance of higher-order quantum operation becomes easier since it is enough to perform an optimization on a restricted set of supermap.

The positivity condition for the Choi operator of a supermap is always necessary if we focus on the ones that are compatible with quantum mechanics. We believe that the developments of methods for utilizing the positivity condition leads to a better understanding and analysis of higher-order quantum operations.

In the second topic, we proposed a consistent definition of the controlled version of general quantum operations based on physical and axiomatic approaches, and then extend the definition to the controlled version of higher-order quantum operations. By utilizing the proposed definitions, we analyzed the problem of controllization and proposed a new quantum algorithm for controllization which requires no auxiliary system. The proposed quantum algorithm for controllization utilizes a randomization based on the Pauli operations. We also evaluated a similar algorithm based on the Clifford operations, and we show that the randomization based on the Pauli operations performs better in our algorithm.

One difference between controllization and other higher-order quantum operations like unitary inversion is that the target operation is not uniquely determined. That is, there is some freedom to define the phase factor of a controlled unitary operation in controllization. Recently, the difficulty of controllization is also analyzed by investigating the topological structure in the freedom of the phase factor [63], and it is shown that exact controllization with multiple uses of an input unitary operation is only possible in a similar method presented in Sec. 4.4.1 under certain assumptions. Meanwhile, the quantum algorithm we proposed in Sec. 4.4.2 implements controllization with an arbitrarily small error if enough division of the input unitary operation is allowed. The phase factor is determined by the trace of the corresponding Hamiltonian, which is well-defined only if an arbitrary division of the unitary operation is possible.

The new quantum algorithm we proposed in Sec. 4.4.2 shows that allowing arbitrary division of the input unitary operation, equivalently considering higher-order quantum operations based on Hamiltonian dynamics instead of unitary operations, presents various advantages. Here, we utilized a structure with repetition to capture the problem within the usual framework of higher-order quantum operations. However, a more general kind of higher-order transformations between Hamiltonian dynamics can be considered, and there is no framework for analyzing this kind of higher-order transformations yet. A general framework for higher-order transformations between Hamiltonian dynamics provides more power for quantum information processing, and it is worth trying to develop such a framework.

In the third topic, we proposed a new structure named success-or-draw for probabilistic higher-order quantum operations, which allows a repeat-until-success implementation of them. With the success-or-draw structure, a probabilistic higher-order quantum operation can amplify its success probability exponentially to one by increasing the number of uses of an input quantum operation. We provided a mathematical formulation and we showed that a large class of probabilistic higher-order quantum operations can incorporate such a structure. In particular, any probabilistic higher-order quantum operation transforming unitary operations into CPTP maps can obtain the success-or-draw structure by adding the number of uses of the unitary operation.

We provided a recipe for constructing the success-or-draw higher-order quantum operations in our proof, but the provided recipe is not efficient in general. In particular, in order to satisfy the positivity condition of the Choi operator, we constructed the Choi operator to be a full-rank operator on a certain subspace. In the unitary inversion, the Choi operator that achieves the optimal success probability, which was obtained numerically, has a lower rank than the one used in our construction. However, it is not obvious if there are other methods for satisfying the positivity condition. It is an open question if there exists a better recipe for constructing a success-or-draw higher-order quantum operations and a universal bound on the change of the probability by requiring the success-or-draw structure.

We hope that our results contribute to the developments of quantum information processing utilizing higher-order quantum operations from both theoretical and experimental aspects.

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Appendix A

Evaluation of the Summation in the Proof of Theorem 3.1

We evaluate the summation $\sum_{J\in G_a\otimes G_b}||\mathrm{Tr}_{in}WJ^t||_1$ for each a,b in the following. Note that it is enough to consider only 6 cases that satisfy $a\le b$ because of the symmetry between the two systems. In the following, when we take summation on J, it also indicates the summation on the corresponding variables in the form $|ijkl\rangle\langle i'j'k'l'|$.

(Case 1: $G_1\otimes G_1$) In this case, the equality

$$\sum_{J\in G_1\otimes G_1}||\mathrm{Tr}_{in}WJ^t||_1=\sum_{J\in G_1\otimes G_1}||\langle ijkl||W\rangle\langle W||i'j'k'l'\rangle||_1 \tag{A.1}$$

$$=\sum_{J\in G_1\otimes G_1}(||\delta_{jk}\delta_{j'k'}|il00\rangle\langle i'l'00|||_1+||\delta_{il}\delta_{i'l'}|kj11\rangle\langle k'j'11|||_1$$
$$+||\delta_{jk}\delta_{i'l'}|il00\rangle\langle k'j'11|||_1+||\delta_{il}\delta_{j'k'}|kj11\rangle\langle i'l'00|||_1), \tag{A.2}$$

holds. Moreover, the summation over the 1st and 2nd terms or the 3rd and 4th terms are equal because of the symmetry, and thus we only evaluate the 1st and 3rd terms here.

For the 1st term of Eq. (A.2), the equality

$$\sum_{J\in G_1\otimes G_1}||\delta_{jk}\delta_{j'k'}|il00\rangle\langle i'l'00|||_1=\sum_{J\in G_1\otimes G_1}\delta_{jk}\delta_{j'k'} \tag{A.3}$$

holds. In order to evaluate the summation, we consider the following two cases. If $j\neq j'$, there are $d(d-1)(d-2)(d-3)+5d(d-1)(d-2)+2d(d-1)$ possible choices on (i,j,i',j') and for each choice of (i,j,i',j'), there are only $(d-2)(d-3)+5(d-2)+2$ possible choices on (k,l,k',l') because $k=j,k'=j'$ is necessary for non-vanishing kronecker delta. Similarly, if $j=j'$, there are $d(d-1)(d-2)$ possible choices on (i,j,i',j') and for each choice of (i,j,i',j'), there are $(d-1)(d-2)$ possible choices on (k,l,k',l'). For the 3rd term of Eq. (A.2), the equality

$$\sum_{J\in G_1\otimes G_1} ||\delta_{jk}\delta_{i'l'}|il00\rangle\langle k'j'11|||_1 = \sum_{J\in G_1\otimes G_1} \delta_{jk}\delta_{i'l'} \tag{A.4}$$

holds. Similarly, if $j\neq i'$, there are $d(d-1)(d-2)(d-3)+5d(d-1)(d-2)+d(d-1)$ possible choices on (i,j,i',j') and for each choice of (i,j,i',j'), there are $(d-2)(d-3)+5(d-2)+1$ possible choices on (k,l,k',l'). If $j=i'$, there are $d(d-1)(d-2)+d(d-1)$ possible choices on (i,j,i',j') and for each choice of (i,j,i',j'), there are $(d-1)(d-2)+(d-1)$ possible choices on (k,l,k',l').

In total, we obtain

$$\begin{aligned}
&\sum_{J\in G_1\otimes G_1} ||\mathrm{Tr}_{in} W J^t||_1 \\
&= 2\sum_{J\in G_1\otimes G_1} \delta_{jk}\delta_{j'k'} + 2\sum_{J\in G_1\otimes G_1} \delta_{jk}\delta_{i'l'} &\text{(A.5)}\\
&= 2d(d-1)(2d^4+2d^3-18d^2+11d+8). &\text{(A.6)}
\end{aligned}$$

(Case 2: $G_1\otimes G_2$) In this case, the equality

$$\begin{aligned}
&\sum_{J\in G_1\otimes G_2} ||\mathrm{Tr}_{in} W J^t||_1 \\
&= \sum_{J\in G_1}\sum_{m=0}^{d-1} ||\sum_{k=0}^{d-1} \langle ijk,k+m||W\rangle\langle W||i'j'k,k+m\rangle||_1 &\text{(A.7)}\\
&= \sum_{J\in G_1}\sum_{m=0}^{d-1} ||\sum_{k=0}^{d-1} (\delta_{jk}\delta_{j'k}|i,k+m,00\rangle\langle i',k+m,00| + \delta_{i,k+m}\delta_{i',k+m}|kj11\rangle\langle kj'11| \\
&\quad + \delta_{jk}\delta_{i',k+m}|i,k+m,00\rangle\langle kj'11| + \delta_{i,k+m}\delta_{j'k}|kj11\rangle\langle i',k+m,00|)||_1 &\text{(A.8)}\\
&= \sum_{J\in G_1}\sum_{m,k} (\delta_{jk}\delta_{j'k} + \delta_{i,k+m}\delta_{i',k+m} + \delta_{jk}\delta_{i',k+m} + \delta_{i,k+m}\delta_{j'k}) &\text{(A.9)}
\end{aligned}$$

holds. The summation over the 1st and 2nd terms or the 3rd and 4th terms are equal, and thus we only evaluate the 1st and 3rd terms here.

The summation over the 1st term of Eq. (A.9) can be evaluated as $d^2(d-1)(d-2)$, because for each $k,m=0,\ldots,d-1$, there are $(d-1)(d-2)$ possible choices on (i,j,i',j') due to $j=j'=k$. The summation over the 3st term of Eq. (A.9) can be evaluated as follows: for each $k=0,\ldots,d-1$, if $m=0$, there are $(d-1)(d-2)+(d-1)$ possible choices on (i,j,i',j'), and if $m\neq 0$, there are $(d-2)(d-3)+5(d-2)+1$ possible choices on (i,j,i',j').

In total, we obtain

$$
\begin{aligned}
&\sum_{J\in G_1\otimes G_2} ||\mathrm{Tr}_{in} W J^t||_1 \\
&= 2\{d^2(d-1)(d-2) + d[(d-1)(d-2)+(d-1)] \\
&\quad + d(d-1)[(d-2)(d-3)+5(d-2)+1]\} && \text{(A.10)} \\
&= 2d(d-1)(2d^2-d-4). && \text{(A.11)}
\end{aligned}
$$

(Case 3: $G_2 \otimes G_2$) In this case, the summation is evaluated as

$$
\begin{aligned}
&\sum_{J\in G_2\otimes G_2} ||\mathrm{Tr}_{in} W J^t||_1 \\
&= \sum_{n,m=0}^{d-1} \sum_{i,k=0}^{d-1} (\delta_{i+n,k}\delta_{i+n,k} + \delta_{i,k+m}\delta_{i,k+m} + \delta_{i+n,k}\delta_{i,k+m} + \delta_{i,k+m}\delta_{i+n,k}) && \text{(A.12)} \\
&= 2\sum_{n,m=0}^{d-1} \sum_{i,k=0}^{d-1} (\delta_{i+n,k}\delta_{i+n,k} + \delta_{i+n,k}\delta_{i,k+m}) && \text{(A.13)} \\
&= 2(d^3+d^2) = 2d^2(d+1). && \text{(A.14)}
\end{aligned}
$$

(Case 4: $G_1 \otimes G_3$) Here we consider G_3 with only the elements of the form $|kl\rangle\langle kk| - |ll\rangle\langle lk|$. The elements of the other form can be evaluated in the same way since the two input systems are symmetric. We denote this group as G_3', that is,

$$
G_3' = \{|kl\rangle\langle kk| - |ll\rangle\langle lk| \mid k \neq l\} \tag{A.15}
$$

and the following equality holds

$$
\sum_{J\in G_1\otimes G_3} ||\mathrm{Tr}_{in} W J^t||_1 = 2 \sum_{J\in G_1\otimes G_3'} ||\mathrm{Tr}_{in} W J^t||_1. \tag{A.16}
$$

In this case, the summation can be evaluated as

$$
\begin{aligned}
\sum_{J\in G_1\otimes G_3'} ||\mathrm{Tr}_{in} W J^t||_1 &= \sum_{J\in G_1}\sum_{k\neq l} ||\langle ijkl||W\rangle\langle W||i'j'kk\rangle - \langle ijll||W\rangle\langle W||i'j'lk\rangle||_1 && \text{(A.17)} \\
&= \sum_{J\in G_1}\sum_{k\neq l} ||(\delta_{jk}\delta_{j'k}|il00\rangle\langle i'k00| - \delta_{jl}\delta_{j'l}|il00\rangle\langle i'k00|) \\
&\quad + (\delta_{il}\delta_{i'k}|kj11\rangle\langle kj'11| - \delta_{il}\delta_{i'k}|lj11\rangle\langle lj'11|) \\
&\quad + (\delta_{jk}\delta_{i'k}|il00\rangle\langle kj'11| - \delta_{jl}\delta_{i'k}|il00\rangle\langle lj'11|) \\
&\quad + (\delta_{il}\delta_{j'k}|kj11\rangle\langle i'k00| - \delta_{il}\delta_{j'l}|lj11\rangle\langle i'k00|)||_1 && \text{(A.18)}
\end{aligned}
$$

$$= \sum_{J\in G_1}\sum_{k\neq l}(||\delta_{jk}\delta_{j'k}|il00\rangle\langle i'k00| - \delta_{jl}\delta_{j'l}|il00\rangle\langle i'k00|||_1$$
$$+ ||\delta_{il}\delta_{i'k}|kj11\rangle\langle kj'11| - \delta_{il}\delta_{i'k}|lj11\rangle\langle lj'11|||_1$$
$$+ ||\delta_{jk}\delta_{i'k}|il00\rangle\langle kj'11| - \delta_{jl}\delta_{i'k}|il00\rangle\langle lj'11|||_1$$
$$+ ||\delta_{il}\delta_{j'k}|kj11\rangle\langle i'k00| - \delta_{il}\delta_{j'l}|lj11\rangle\langle i'k00|||_1) \tag{A.19}$$
$$= \sum_{J\in G_1}\sum_{k\neq l}(\delta_{jk}\delta_{j'k} + \delta_{jl}\delta_{j'l} + 2\delta_{il}\delta_{i'k} + \delta_{jk}\delta_{i'k} + \delta_{jl}\delta_{i'k} + \delta_{il}\delta_{j'k} + \delta_{il}\delta_{j'l}) \tag{A.20}$$
$$= 2\sum_{J\in G_1}\sum_{k\neq l}(\delta_{jk}\delta_{j'k} + \delta_{il}\delta_{i'k} + \delta_{jk}\delta_{i'k} + \delta_{jl}\delta_{i'k}), \tag{A.21}$$

where the third equality holds because the states of control qubits are different, the forth equality holds because $k \neq l$, and the last equality holds because the summation over the 1st and 2nd, 4th and 7th, 5th and 6th terms are the same respectively. For each (k, l), by counting the number of possible choices of (i, j, i', j'), we obtain

$$\sum_{J\in G_1\otimes G_3'} ||\mathrm{Tr}_{in}WJ^t||_1$$
$$= 2d(d-1)\sum_{J\in G_1}(\delta_{jk}\delta_{j'k} + \delta_{il}\delta_{i'k} + \delta_{jk}\delta_{i'k} + \delta_{jl}\delta_{i'k}), \tag{A.22}$$
$$= 2d(d-1) \times \{[(d-1)(d-2)] + [(d-2)(d-3) + 5(d-2) + 2]$$
$$+ [(d-1)(d-2) + (d-1)] + [(d-2)(d-3) + 5(d-2) + 1]\} \tag{A.23}$$
$$= 2d(d-1)(4d^2 - 5d - 2), \tag{A.24}$$

and thus, we obtain

$$\sum_{J\in G_1\otimes G_3} ||\mathrm{Tr}_{in}WJ^t||_1 = 4d(d-1)(4d^2 - 5d - 2). \tag{A.25}$$

(Case 5: $G_2 \otimes G_3$) As in the case 4, we consider G_3' instead, and using the following equality:

$$\sum_{J\in G_2\otimes G_3} ||\mathrm{Tr}_{in}WJ^t||_1 = 2\sum_{J\in G_2\otimes G_3'} ||\mathrm{Tr}_{in}WJ^t||_1. \tag{A.26}$$

In this case, the summation can be evaluated as

$$\sum_{J\in G_2\otimes G_3'} ||\mathrm{Tr}_{in}WJ^t||_1 = \sum_{k\neq l}\sum_{m=0}^{d-1}||\sum_{i=0}^{d-1}(\langle i, i+m, kl||W\rangle\langle W||i, i+m, kk\rangle$$
$$- \langle i, i+m, ll||W\rangle\langle W||i, i+m, lk\rangle)||_1 \tag{A.27}$$

$$= \sum_{k\neq l}\sum_{m=0}^{d-1}||\sum_{i=0}^{d-1}\delta_{i+m,k}\delta_{i+m,k}|il00\rangle\langle ik00| - \delta_{i+m,l}\delta_{i+m,l}|il00\rangle\langle ik00|||_1$$
$$+ ||\sum_{i}\delta_{il}\delta_{ik}|k,i+m,11\rangle\langle k,i+m,11| - \delta_{il}\delta_{ik}|l,i+m,11\rangle\langle l,i+m,11|||_1$$
$$+ ||\sum_{i}\delta_{i+m,k}\delta_{ik}|il00\rangle\langle k,i+m,11| - \delta_{i+m,l}\delta_{ik}|il00\rangle\langle l,i+m,11|||_1$$
$$+ ||\sum_{i}\delta_{il}\delta_{i+m,k}|k,i+m,11\rangle\langle ik00| - \delta_{il}\delta_{i+m,l}|l,i+m,11\rangle\langle ik00|||_1 \quad \text{(A.28)}$$
$$= \sum_{k\neq l}\sum_{m,i=0}^{d-1}(\delta_{i+m,k}\delta_{i+m,k} + \delta_{i+m,l}\delta_{i+m,l} + \delta_{il}\delta_{ik} + \delta_{il}\delta_{ik}$$
$$+ \delta_{i+m,k}\delta_{ik} + \delta_{i+m,l}\delta_{ik} + \delta_{il}\delta_{i+m,k} + \delta_{il}\delta_{i+m,l}) \quad \text{(A.29)}$$
$$= d(d-1)\times[d+d+0+0+1+1+1+1] \quad \text{(A.30)}$$
$$= 2d(d-1)(d+2). \quad \text{(A.31)}$$

Here, the second equality holds because the states of control qubits are different, the third equality holds because $k \neq l$, and the fourth equality holds by counting the number of possible choices of (i, j, i', j') for each (k, l). In total, we obtain

$$\sum_{J\in G_2\otimes G_3}||\mathrm{Tr}_{in}WJ^t||_1 = 4d(d-1)(d+2). \quad \text{(A.32)}$$

(Case 6: $G_3 \otimes G_3$) In this case, we divide the first G_3 into two groups, i.e., G_3' and G_3'', where G_3' defined by Eq. (A.15) is the one used in cases 4 and 5, and G_3'' is defined as the remaining of G_3, that is,

$$G_3'' = \{|ji\rangle\langle ii| - |jj\rangle\langle ij| \mid i \neq j\}. \quad \text{(A.33)}$$

Here we evaluate both $G_3' \otimes G_3'$ and $G_3'' \otimes G_3'$, and the result can be obtained by

$$\sum_{J\in G_3\otimes G_3}||\mathrm{Tr}_{in}WJ^t||_1 = 2(\sum_{J\in G_3'\otimes G_3'}||\mathrm{Tr}_{in}WJ^t||_1 + \sum_{J\in G_3''\otimes G_3'}||\mathrm{Tr}_{in}WJ^t||_1). \quad \text{(A.34)}$$

We first consider the summation over $G_3' \otimes G_3'$, which is evaluated as

$$\sum_{J\in G_3'\otimes G_3'}||\mathrm{Tr}_{in}WJ^t||_1$$
$$= \sum_{i\neq j}\sum_{k\neq l}||\langle ijkl||W\rangle\langle W||iikk\rangle - \langle ijll||W\rangle\langle W||iilk\rangle$$
$$- \langle jjkl||W\rangle\langle W||jikk\rangle + \langle jjll||W\rangle\langle W||jilk\rangle||_1 \quad \text{(A.35)}$$

$$= \sum_{i\neq j,k\neq l} ||(\delta_{jk}\delta_{ik} - \delta_{jl}\delta_{il})|il00\rangle\langle ik00| - (\delta_{jk}\delta_{ik} - \delta_{jl}\delta_{il})|jl00\rangle\langle jk00|)||_1$$
$$+ ||(\delta_{il}\delta_{ik} - \delta_{jl}\delta_{jk})|kj11\rangle\langle ki11| - (\delta_{il}\delta_{ik} - \delta_{jl}\delta_{jk})|lj11\rangle\langle li11|)||_1$$
$$+ ||(\delta_{jk}\delta_{ik}|il00\rangle\langle ki11| - \delta_{jl}\delta_{ik}|il00\rangle\langle li11| - \delta_{jk}\delta_{jk}|jl00\rangle\langle ki11| + \delta_{jl}\delta_{jk}|jl00\rangle\langle li11|)||_1$$
$$+ ||(\delta_{il}\delta_{ik}|kj11\rangle\langle ik00| - \delta_{il}\delta_{il}|lj11\rangle\langle ik00| - \delta_{jl}\delta_{ik}|kj11\rangle\langle jk00| + \delta_{jl}\delta_{il}|lj11\rangle\langle jk00|||_1 \tag{A.36}$$
$$= \sum_{i\neq j,k\neq l} 3\delta_{jk}\delta_{ik} + 3\delta_{jl}\delta_{il} + 3\delta_{il}\delta_{ik} + 3\delta_{jl}\delta_{jk} + 2\delta_{jl}\delta_{ik} + \delta_{jk}\delta_{jk} + \delta_{il}\delta_{il} \tag{A.37}$$
$$= \sum_{i\neq j,k\neq l} 2\delta_{jl}\delta_{ik} + \delta_{jk}\delta_{jk} + \delta_{il}\delta_{il} \tag{A.38}$$
$$= 2d(d-1) + 2d(d-1)^2 = 2d^2(d-1), \tag{A.39}$$

where the second equality holds because the states of control qubits are different, and the third equality holds because $i \neq j$ and $k \neq l$. Similarly, the summation over $G_3'' \otimes G_3'$ can be evaluated as

$$\sum_{J\in G_3''\otimes G_3'} ||\mathrm{Tr}_{in} W J^t||_1$$
$$= \sum_{i\neq j,k\neq l} ||\langle jikl||W\rangle\langle W||iikk\rangle - \langle jill||W\rangle\langle W||iilk\rangle$$
$$- \langle jjkl||W\rangle\langle W||ijkk\rangle + \langle jjll||W\rangle\langle W||ijlk\rangle||_1 \tag{A.40}$$
$$= \sum_{i\neq j,k\neq l} ||(\delta_{ik}\delta_{ik} - \delta_{il}\delta_{il} - \delta_{jk}\delta_{jk} + \delta_{jl}\delta_{jl})|jl00\rangle\langle ik00|)||_1$$
$$+ ||(\delta_{jl}\delta_{ik}|ki11\rangle\langle ki11| - \delta_{jl}\delta_{ik}|li11\rangle\langle li11| - \delta_{jl}\delta_{ik}|kj11\rangle\langle kj11| + \delta_{jl}\delta_{ik}|lj11\rangle\langle lj11|)||_1$$
$$+ ||(\delta_{ik}\delta_{ik}|jl00\rangle\langle ki11| - \delta_{il}\delta_{ik}|jl00\rangle\langle li11| - \delta_{jk}\delta_{ik}|jl00\rangle\langle kj11| + \delta_{jl}\delta_{ik}|jl00\rangle\langle lj11|)||_1$$
$$+ ||(\delta_{jl}\delta_{ik}|ki11\rangle\langle ik00| - \delta_{jl}\delta_{il}|li11\rangle\langle ik00| - \delta_{jl}\delta_{jk}|kj11\rangle\langle ik00| + \delta_{jl}\delta_{jl}|lj11\rangle\langle ik00|||_1 \tag{A.41}$$
$$= \sum_{i\neq j,k\neq l} 2\delta_{ik}\delta_{ik} + \delta_{il}\delta_{il} + \delta_{jk}\delta_{jk} + 2\delta_{jl}\delta_{jl}$$
$$+ 4\delta_{jl}\delta_{ik} + \delta_{il}\delta_{ik} + \delta_{jk}\delta_{ik} + 2\delta_{jl}\delta_{ik} + \delta_{jl}\delta_{il} + \delta_{jl}\delta_{jk} \tag{A.42}$$
$$= \sum_{i\neq j,k\neq l} 4\delta_{jl}\delta_{ik} + 2\delta_{ik}\delta_{ik} + 2\delta_{jl}\delta_{jl} + 2\delta_{jl}\delta_{ik} + \delta_{il}\delta_{il} + \delta_{jk}\delta_{jk} \tag{A.43}$$
$$= d(d-1)[4 + 2(d-1) + 2(d-1) + 2 + (d-1) + (d-1)] \tag{A.44}$$
$$= 6d^2(d-1) \tag{A.45}$$

where the second equality holds because the states of control qubits are different. For the third equality, the expansion can be done for all but the first term using $i \neq j$ and $k \neq l$. For the first term, there exists some patterns where more than one terms of kronecker deltas are non-zero, for example, $\delta_{ik}\delta_{ik}$ and $\delta_{jl}\delta_{jl}$ can be non-zero simultaneously. However, since they have same sign, the expansion is possible and the third equality holds.

In total, we obtain

$$\sum_{J\in G_3\otimes G_3} ||\mathrm{Tr}_{in} W J^t||_1 = 16d^2(d-1). \tag{A.46}$$

Finally, we have evaluated all terms in Eq. (3.83), and we obtain

$$||W||_1 \geq (2d^3)^2, \tag{A.47}$$

which completes the prove of Theorem 3.1.

Appendix B

The Kraus Representation for Quantum Combs

For the completeness, we derive the conditions for an N-slot quantum comb $\widetilde{\mathcal{S}} : \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_{2N}) \to \mathcal{L}(\mathcal{H}_0 \otimes \mathcal{H}_{2N+1})$ in terms of the Kraus representation, instead of the Choi representation. Let $\{K_i\}$ be the Kraus operators of $\widetilde{\mathcal{S}}$, that is,

$$\widetilde{\mathcal{S}}(J) = \sum_i K_i J K_i^\dagger, \tag{B.1}$$

with $K_i \in \mathcal{L}(\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_{2N}, \mathcal{H}_0 \otimes \mathcal{H}_{2N+1})$. Since the positivity condition of a quantum comb given by Eq. (4.40) is automatically satisfied, the remaining condition to be derived is the causal condition given by Eq. (4.41).

We first consider the causal condition given by Eq. (4.41) for $k = N$, that is,

$$\mathrm{Tr}_{2N+1} S = (\mathrm{Tr}_{2N,2N+1} S) \otimes \frac{I_{2N}}{d_{2N}}. \tag{B.2}$$

In order to rewrite this condition, we first consider the following condition which is equivalent to Eq. (B.2), that is, the equality

$$\begin{aligned}
&\mathrm{Tr}_{0;2N-1}(A_0 \otimes B_{1;2N-1} \otimes I_{2N}) \mathrm{Tr}_{2N+1} S \\
&= \mathrm{Tr}_{0;2N-1}(A_0 \otimes B_{1;2N-1} \otimes I_{2N}) \mathrm{Tr}_{2N,2N+1} S \otimes \frac{I_{2N}}{d_{2N}} \\
&= c \cdot I_{2N}
\end{aligned} \tag{B.3}$$

holds for any $A_0 \in \mathcal{L}(\mathcal{H}_0)$ and $B_{1;2N-1} \in \mathcal{L}(\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_{2N-1})$ and a complex number depending on $A_0, B_{1;2N_1}$, where $\mathrm{Tr}_{0;2N-1}$ denotes the partial trace taken over $\mathcal{H}_0 \otimes \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_{2N-1}$. By rewriting the Choi operator S in terms of the

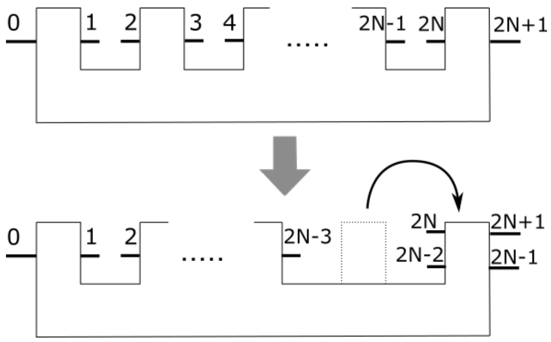

Figure B.1: (Above) An N-slot quantum comb $\widetilde{\mathcal{S}}$ which takes N quantum operations $\widetilde{\mathcal{A}}_k$ for $k = 1, 2, \cdots, N$ as input operation. (Below) The $(N-1)$-slot quantum comb $\widetilde{\mathcal{S}}^{(1)} : \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes (\mathcal{H}_{2N-2} \otimes \mathcal{H}_{2N})) \to \mathcal{L}(\mathcal{H}_0 \otimes (\mathcal{H}_{2N-1} \otimes \mathcal{H}_{2N+1}))$ induced from the N-slot quantum comb $\widetilde{\mathcal{S}}$. The $(N-k)$-slot quantum comb $\widetilde{\mathcal{S}}^{(k)}$ for $k = 1, 2, \cdots, N-1$ is defined by repeating this procedure.

Kraus operators $\{K_i\}$, we obtain an equivalent condition, that is, the equality

$$\begin{aligned}&\mathrm{Tr}_{0;2N-1}(A_0 \otimes B_{1;2N-1} \otimes I_{2N})\mathrm{Tr}_{2N+1}S \\ &= \sum_{k,k'} |k\rangle\langle k'|_{2N} \cdot \mathrm{Tr}_{2N}\big[|k\rangle\langle k'|_{2N}\mathrm{Tr}_{1;2N-1}(B_{1;2N-1} \otimes I_{2N}) \sum_i K_i^\dagger (A_0 \otimes I_{2N+1}) K_i\big],\end{aligned} \tag{B.4}$$

holds for any $A_0 \in \mathcal{L}(\mathcal{H}_0)$ and $B_{1;2N-1} \in \mathcal{L}(\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_{2N-1})$. Thus, we obtain the condition in terms of the Kraus operators $\{K_i\}$, namely, for any linear operators $A_0 \in \mathcal{L}(\mathcal{H}_0)$ and $B_{1;2N-1} \in \mathcal{L}(\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_{2N-1})$, the following equality holds

$$\mathrm{Tr}_{1;2N-1}[(B_{1;2N-1} \otimes I_{2N}) \sum_i K_i^\dagger (A_0 \otimes I_{2N+1}) K_i] = c \cdot I_{2N}, \tag{B.5}$$

where c is a complex number given by the trace of the l.h.s. divided by d_{2N}.

An N-slot quantum comb $\widetilde{\mathcal{S}}$ can be redefined as an (N-1)-slot quantum comb denoted by $\widetilde{\mathcal{S}}^{(1)} : \mathcal{L}(\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_{2N-4} \otimes \mathcal{H}'_{2N-2}) \to \mathcal{L}(\mathcal{H}_0 \otimes \mathcal{H}'_{2N-1})$ with $\mathcal{H}'_{2N-2} = \mathcal{H}_{2N-2} \otimes \mathcal{H}_{2N}$ and $\mathcal{H}'_{2N-1} = \mathcal{H}_{2N-1} \otimes \mathcal{H}_{2N+1}$, as shown in Fig. B.1. The corresponding Kraus operators $\{K_i^{(1)}\}$ are given as

$$K_i^{(1)} = K_i |I_{2N-1}\rangle\rangle_{2N-1,2N-1}, \tag{B.6}$$

where $K_i^{(1)}$ can be understood as the operator K_i with its domain $\mathcal{H}_{2N-1}$ been moved to the range. Recursively, we can define an (N-k)-slot quantum combs $\widetilde{\mathcal{S}}^{(k)}$, and its Kraus operators $\{K_i^{(k)}\}$ of $\widetilde{\mathcal{S}}^{(k)}$ are given as

$$K_i^{(k)} = K_i |I_{2N-2k+1}\rangle\rangle \otimes |I_{2N-2k+3}\rangle\rangle \otimes \cdots \otimes |I_{2N-1}\rangle\rangle. \tag{B.7}$$

We also let $\widetilde{\mathcal{S}}^{(0)} = \widetilde{\mathcal{S}}$ and $K_i^{(0)} = K_i$.

Then the condition Eq. (B.5) can be transformed to the condition for $\widetilde{\mathcal{S}}^{(k)}$ with $k = 0, 1, \ldots, N-1$, which correspond to the condition Eq. (4.41) with $N-k$, as shown in the following. Note that Eq. (B.5) corresponds to the case of $k = 0$. For all liner operators A_0 and $B_{1;2N-2k-1}$, there is a complex number c such that

$$\mathrm{Tr}_{1;2N-2k-1}[(B_{1;2N-2k-1} \otimes I_{\mathcal{H}^{(k)}}) \sum_i K_i^{(k)\dagger}(A_0 \otimes I_{\mathcal{K}^{(k)}})K_i^{(k)}] = c \cdot I_{\mathcal{H}^{(k)}}, \quad \text{(B.8)}$$

with $\mathcal{H}^{(k)} = \bigotimes_{l=0}^{k} \mathcal{H}_{2N-2l}, \mathcal{K}^{(k)} = \bigotimes_{l=0}^{k} \mathcal{H}_{2N-2l+1}$. The remaining condition given by Eq. (4.41) is the one for $k = 0$, and it is equivalent to

$$\mathrm{Tr}_{\mathcal{K}^{(N)}} S = I_{\mathcal{H}^{(N)}}, \quad \text{(B.9)}$$

when all other conditions given by Eq. (4.41) are satisfied. Since this condition is similar to the TP condition of a map from $\mathcal{H}^{(N)}$ to $\mathcal{K}^{(N)}$, it can be written with $\langle\langle I_0|K_i^{(N)}$ as $\sum_i K_i^{(N)\dagger}|I_0\rangle\rangle\langle\langle I_0|S_i^{(N)} = I_{\mathcal{H}^{(N)}}$, equivalently, we obtain

$$\mathrm{Tr}_{\mathcal{K}^{(N)}} \sum_i K_i^{\dagger}(|I_0\rangle\rangle\langle\langle I_0|_{0,0} \otimes I_{2N+1})K_i = I_{\mathcal{H}^{(N)}}. \quad \text{(B.10)}$$

As the positivity of the quantum comb Eq. (4.40) is automatically satisfied, the condition for quantum comb in terms of the Kraus representation is given by Eq. (B.8) with $k = 0, 1, \ldots, N-1$ and Eq. (B.10).

Appendix C

The Proof of Theorem 5.1

We first clarify the notations. Let $d := d_{\mathcal{I}_i} = d_{\mathcal{O}_j}$ for $i, j \geq 1$, and $d_0 := d_{\mathcal{I}_0} = d_{\mathcal{O}_0}$. For Lemma C.1, we define the following operators. Note that we consider the case where K uses of an input unitary operation is allowed in Lemma C.1. We first define the permutation operator $P_\sigma^{\mathcal{I}}$ and $P_\sigma^{\mathcal{O}}$ that permute systems $\mathcal{I} = \mathcal{I}_1\mathcal{I}_2\cdots\mathcal{I}_K$ and $\mathcal{O} = \mathcal{O}_1\mathcal{O}_2\cdots\mathcal{O}_K$ according to the permutation σ. The permutation of input operations is given by $P_\sigma^{\mathcal{IO}} := P_\sigma^{\mathcal{I}} \otimes P_\sigma^{\mathcal{O}}$, which simultaneously permute the input system and the output system of a single input operation according to the permutation σ. The symmetric subspace of input operations $\Pi_{sym}^{\mathcal{IO}}$ is given by

$$\Pi_{sym}^{\mathcal{IO}} := \sum_\sigma P_\sigma^{\mathcal{IO}} = \sum_\sigma P_\sigma^{\mathcal{I}} \otimes P_\sigma^{\mathcal{O}}. \tag{C.1}$$

For Lemma C.2, we define a set of Hermitian operators $\{g_i\}_{i=0}^{d^2-1}$ that forms the operator basis for d-dimensional Hermitian operators, with $g_0 = I_d$, others being traceless, and the orthogonality $\mathrm{Tr} g_i g_j = d\delta_{ij}$ holds [64]. For example, the Pauli matrices for $d = 2$, and Gell-Mann matrices for $d = 3$ are these sets of Hermitian operators. We also define the set for d_0-dimensional Hermitian operators as $\{h_i\}_{i=0}^{d_0^2-1}$. In Lemma C.2, we rewrite the condition that a comb transforms unitary operations to CPTP maps in terms of the Choi operator and the Hermitian operator basis.

In order to prove Theorem 5.1, we first consider Lemma C.1 and Lemma C.2, which shows that it is enough to prove another theorem given as Theorem C.1.

Lemma C.1. *If* $\mathrm{Tr}_{\mathcal{IO}}(\Pi_{sym}^{\mathcal{IO}} N \Pi_{sym}^{\mathcal{IO}}) \propto J_{id}$, *then* N *neutralizes all unitary operations as* $\widetilde{\widetilde{\mathcal{N}}}(\widetilde{\mathcal{U}}^{\otimes K}) \propto \widetilde{id}$.

Proof. Note that the if condition is equivalent to $\mathrm{Tr}_{\mathcal{IO}}(\Pi_{sym}^{\mathcal{IO}} N \Pi_{sym}^{\mathcal{IO}}) \leq d^K J_{id}$, due to the normalization condition $\mathrm{Tr} N \leq d^K d_0$.

For any input channel J_U, ${J_U}^{\otimes K} \leq d^K I$ holds and $A := d^K I - {J_U}^{\otimes K} \geq 0$. Thus

$$
\begin{aligned}
J_{id} &\geq \mathrm{Tr}_{\mathcal{IO}}[(\Pi_{sym}^{\mathcal{IO}} N \Pi_{sym}^{\mathcal{IO}})/d^K] && \text{(C.2)}\\
&= \mathrm{Tr}_{\mathcal{IO}}[(\Pi_{sym}^{\mathcal{IO}} N \Pi_{sym}^{\mathcal{IO}})(A + {J_U}^{\otimes K})]/d^{2K} && \text{(C.3)}\\
&= \mathrm{Tr}_{\mathcal{IO}}[(\Pi_{sym}^{\mathcal{IO}} N \Pi_{sym}^{\mathcal{IO}})A + \mathrm{Tr}_{\mathcal{IO}}(\Pi_{sym}^{\mathcal{IO}} N \Pi_{sym}^{\mathcal{IO}}){J_U}^{\otimes K}]/d^{2K}. && \text{(C.4)}
\end{aligned}
$$

Since the l.h.s is a rank-1 operator, the operators in the r.h.s. are positive, and ${J_U}^{\otimes K}$ is in the symmetric subspace, namely, ${J_U}^{\otimes K} = \Pi_{sym}^{\mathcal{IO}} {J_U}^{\otimes K} \Pi_{sym}^{\mathcal{IO}}$, we obtain

$$
\mathrm{Tr}_{\mathcal{IO}}[N({J_U}^{\otimes K})^T] = \mathrm{Tr}_{\mathcal{IO}}[(\Pi_{sym}^{\mathcal{IO}} N \Pi_{sym}^{\mathcal{IO}})({J_U}^{\otimes K})^T \propto J_{id}, \tag{C.5}
$$

that is, $\widetilde{\widetilde{\mathcal{N}}}(\widetilde{\mathcal{U}}^{\otimes K}) \propto \widetilde{id}$. □

Lemma C.2. *If a one-slot probabilistic comb $S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1\mathcal{O}_0}$ transforms unitary operations to CPTP maps, then $S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} := \mathrm{Tr}_{\mathcal{O}_0} S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1\mathcal{O}_0}$ has a decomposition satisfying*

$$
\begin{aligned}
S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} = \frac{I^{\mathcal{I}_0}}{d_0} \otimes \mathrm{Tr}_{\mathcal{I}_0} S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} &+ \sum_{i=1}^{d_0^2-1}\sum_{j=1}^{d^2-1} \alpha_{ij} h_i^{\mathcal{I}_0} \otimes [g_j^{\mathcal{I}_1} \otimes I^{\mathcal{O}_1}]\\
&+ \sum_{i=1}^{d_0^2-1}\sum_{j=1}^{d^2-1} \beta_{ij} h_i^{\mathcal{I}_0} \otimes [I^{\mathcal{I}_1} \otimes g_j^{\mathcal{O}_1}],
\end{aligned} \tag{C.6}
$$

where $\{\alpha_{ij}\}$ and $\{\beta_{ij}\}$ are real coefficients.

Proof. The Choi operator $S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1}$ can always be decomposed as

$$
\begin{aligned}
S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} = \frac{I^{\mathcal{I}_0}}{d_0} \otimes \mathrm{Tr}_{\mathcal{I}_0} S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} &+ \sum_{i=1}^{d_0^2-1}\sum_{j=1}^{d^2-1} \alpha_{ij} h_i^{\mathcal{I}_0} \otimes [g_j^{\mathcal{I}_1} \otimes I^{\mathcal{O}_1}]\\
+ \sum_{i=1}^{d_0^2-1}\sum_{j=1}^{d^2-1} \beta_{ij} h_i^{\mathcal{I}_0} \otimes [I^{\mathcal{I}_1} \otimes g_j^{\mathcal{O}_1}] &+ \sum_{i=1}^{d_0^2-1}\sum_{j,k=1}^{d^2-1} \gamma_{ijk} h_i^{\mathcal{I}_0} \otimes [g_j^{\mathcal{I}_1} \otimes g_k^{\mathcal{O}_1}],
\end{aligned} \tag{C.7}
$$

and it is enough to show that $\gamma_{ijk} = 0$ for all $i, j, k \geq 1$.

From the assumption, $\mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1}[S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1\mathcal{O}_0}(J_U^T)^{\mathcal{I}_1\mathcal{O}_1}]$ is proportional to the Choi operator of a CPTP map, which satisfies

$$
\mathrm{Tr}_{\mathcal{O}_0}\mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1}[S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1\mathcal{O}_0}(J_U^T)^{\mathcal{I}_1\mathcal{O}_1}] \propto I^{\mathcal{I}_0} \tag{C.8}
$$

where I is the partial trace of the Choi operator of a CPTP map. Thus, $S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1}$ satisfies

$$\mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1}[S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1}(J_U^T)^{\mathcal{I}_1\mathcal{O}_1}] \propto I^{\mathcal{I}_0}. \tag{C.9}$$

Moreover, for any operator O in the linear span of $\mathrm{span}\{J_U\} := \{O \mid O = \sum_i c_i J_{U_i}, c_i \in \mathbb{C}\}$, the condition

$$\mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1}[S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1}(O^T)^{\mathcal{I}_1\mathcal{O}_1}] \propto I^{\mathcal{I}_0} \tag{C.10}$$

holds because of the linearity.

Next, we show that $g_j \otimes g_k \in \mathrm{span}\{J_U\}$ for all $j, k \geq 1$ are in the linear span of $\mathrm{span}\{J_U\}$. From Lemma C.3 shown below, the dimension of the linear span is given by $\dim \mathrm{span}\{J_U\} = (d^2-1)^2 + 1$, and one basis for this span is given by $g_j \otimes g_k$ with $j, k \geq 0$. Note that $g_0 = I_d$. On the other hand, $g_i \otimes I$ and $I \otimes g_i$ for $i \geq 1$ are not in $\mathrm{span}\{J_U\}$, because of the TP property and the unitality of unitary operations, respectively. Thus, the remaining $d^4 - 2(d^2-1) = (d^2-1)^2+1$ elements, especially $g_j \otimes g_k$ with $j, k \geq 1$ and $I \otimes I$, are in the linear span of $\mathrm{span}\{J_U\}$.

Since $g_j \otimes g_k \in \mathrm{span}\{J_U\}$ for all $j, k \geq 1$, by substituting $S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1}$ with the decomposition Eq. (C.7), we obtain $\sum_i \gamma_{ijk} h_i^{\mathcal{I}_0} \propto I^{\mathcal{I}_0}$ for all $j, k \geq 1$. Thus, $\gamma_{ijk} = 0$ is required for all $i, j, k \geq 1$, which proves the Lemma.

□

Lemma C.3. *The dimension of the linear span of* $\mathrm{span}\{J_U\} := \{O \mid O = \sum_i c_i J_{U_i}, c_i \in \mathbb{C}\}$ *is* $(d^2-1)^2 + 1$.

Proof. The vectorization of $J_U = |U\rangle\!\rangle\langle\!\langle U| = (U \otimes I)|I\rangle\!\rangle\langle\!\langle I|(U^\dagger \otimes I)$ is given by $(U^\dagger \otimes I)^T|I\rangle\!\rangle \otimes (U \otimes I)|I\rangle\!\rangle = |U^*\rangle\!\rangle \otimes |U\rangle\!\rangle$, and the dimension of $\mathrm{span}\{J_U\}$ is equivalent to the dimension of $\mathrm{span}\{|U^*\rangle\!\rangle \otimes |U\rangle\!\rangle\} := \{O \mid O = \sum_i c_i |U^*\rangle\!\rangle \otimes |U\rangle\!\rangle, c_i \in \mathbb{C}\}$. In order to obtain the dimension, we consider the projector of $|U^*\rangle\!\rangle \otimes |U\rangle\!\rangle$, and integrate over all unitary operations U as

$$Q = \int dU (|U^*\rangle\!\rangle\langle\!\langle U^*| \otimes |U\rangle\!\rangle\langle\!\langle U|). \tag{C.11}$$

Then the dimension is given by the rank of Q. Consider the substitution of $U \to VU$ with arbitrary V and the invariance of the Haar measure, Q satisfies

$$\begin{aligned} Q &= \int dU (V^* \otimes I \otimes V \otimes I)(|U^*\rangle\!\rangle\langle\!\langle U^*| \otimes |U\rangle\!\rangle\langle\!\langle U|)(V^T \otimes I \otimes V^\dagger \otimes I) && \text{(C.12)} \\ &= (V^* \otimes I \otimes V \otimes I) Q (V^T \otimes I \otimes V^\dagger \otimes I). && \text{(C.13)} \end{aligned}$$

For convenience, we denote the space that V and V^* acting on by A and the remaining by B, then Q satisfies the commutation relation

$$[Q, (U^* \otimes U)^A \otimes I^B] = 0 \tag{C.14}$$

for all unitary operators U. The irreducible representation of $(U^* \otimes U)$ is given by

$$U^* \otimes U = U_1 \oplus U_2, \tag{C.15}$$

where the corresponding dimensions are given by $d_1 = d^2 - 1$ and $d_2 = 1$ for U_1 and U_2 respectively, and the projectors onto the corresponding subspaces are $P_1 := I - \phi^+$ and $P_2 := \phi^+$. From Schur's lemma, Q can be decomposed as

$$Q = \sum_{k=1}^{2} P_k^A \otimes Q_k^B, \tag{C.16}$$

and since P_k^A are projectors, Q is evaluated as

$$Q = \sum_{k=1}^{2} \frac{P_k^A}{d_k} \otimes \mathrm{Tr}_A[(P_k^A \otimes I^B)Q] \tag{C.17}$$

$$= \sum_{k=1}^{2} \frac{P_k^A}{d_k} \otimes \mathrm{Tr}_A[(P_k^A \otimes I^B)|Q'\rangle\rangle\langle\langle Q'|^{AB}], \tag{C.18}$$

where $|Q'\rangle\rangle\langle\langle Q'|^{AB}$ is an arbitrary maximally entangled state between A and B. The second equality holds because of the partial trace on A. Let the maximally entangled state $|Q'\rangle\rangle^{AB}$ be

$$|Q'\rangle\rangle^{AB} = \sum_{l=1}^{2} \sum_{\alpha=0}^{d_l - 1} |l, \alpha\rangle^A \otimes |l, \alpha\rangle^B \tag{C.19}$$

where $l = 1, 2$ are the label for the irreducible representations and α for the basis in P_l. Note that there is no multiplicity subspace in this case. Then

$$(P_k^A \otimes I^B)|Q'\rangle\rangle^{AB} = \sum_{\alpha=0}^{d_k - 1} |k, \alpha\rangle^A \otimes |k, \alpha\rangle^B, \tag{C.20}$$

$$\mathrm{Tr}_A[(P_k^A \otimes I^B)|Q'\rangle\rangle\langle\langle Q'|^{AB}] = P_k^B, \tag{C.21}$$

and thus Q can be written as

$$Q = \sum_{k=1}^{2} \frac{1}{d_k} P_k^A \otimes P_k^B = \frac{1}{d^2 - 1} P_1^A \otimes P_1^B + P_2^A \otimes P_2^B. \tag{C.22}$$

The rank of Q is $(d^2-1)^2+1$, and thus the dimension of $\mathrm{span}\{J_U\}$ is $(d^2-1)^2+1$. □

By considering Lemma C.1 and Lemma C.2, it is enough to prove the following Theorem C.1 in order to prove Theorem 5.1.

Theorem C.1. *Given a one-slot probabilistic comb* $S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1\mathcal{O}_0}$ *with* $\dim\mathcal{I}_1 = \dim\mathcal{O}_1 = d$ *and* $\dim\mathcal{I}_0 = \dim\mathcal{O}_0 = d_0$*. If* $S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} := \mathrm{Tr}_{\mathcal{O}_0} S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1\mathcal{O}_0}$ *has a decomposition satisfying*

$$S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} = \frac{I^{\mathcal{I}_0}}{d_0} \otimes \mathrm{Tr}_{\mathcal{I}_0} S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} + \sum_{i=1}^{d_0^2-1}\sum_{j=1}^{d^2-1} \alpha_{ij} h_i^{\mathcal{I}_0} \otimes [g_j^{\mathcal{I}_1} \otimes I^{\mathcal{O}_1}] + \sum_{i=1}^{d_0^2-1}\sum_{j=1}^{d^2-1} \beta_{ij} h_i^{\mathcal{I}_0} \otimes [I^{\mathcal{I}_1} \otimes g_j^{\mathcal{O}_1}] \tag{C.23}$$

with coefficients $\{\alpha_{ij}\}$ *and* $\{\beta_{ij}\}$*, then there exists* $\varepsilon > 0$ *and a* d*-slot comb* $C = S + N$ *satisfying*

$$\mathrm{Tr}_{\mathcal{I}\mathcal{O}}[S(J_U^{\otimes d})^T] = \varepsilon \mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1}[S_t J_U^T] \tag{C.24}$$

$$\mathrm{Tr}_{\mathcal{I}\mathcal{O}}(\Pi_{sym}^{\mathcal{I}\mathcal{O}} N \Pi_{sym}^{\mathcal{I}\mathcal{O}}) \propto J_{id}. \tag{C.25}$$

The proof of Theorem C.1 consists two parts: the first part presents the construction of $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}} := \mathrm{Tr}_{\mathcal{O}_0} N$; the second part presents the construction of N from $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$ by applying Lemma C.4 shown below.

Proof of Theorem C.1. Let the Choi operator S corresponds to success be

$$S := \varepsilon S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1\mathcal{O}_0} \otimes \frac{I^{\mathcal{I}_2\mathcal{O}_2}}{d} \otimes \cdots \otimes \frac{I^{\mathcal{I}_d\mathcal{O}_d}}{d}. \tag{C.26}$$

Then the condition $S \geq 0$ and Eq. (C.24) is satisfied. The remaining conditions can be classified into the positivity condition $N \geq 0$, the causal condition that $C = S + N$ is a deterministic comb, and the neutralization condition Eq. (C.25).

We first show the idea to construct N satisfying the causal condition. One candidate of the Choi operator corresponding to failure, i.e. a Choi operator satisfies the causal condition that $C = S + F$ is a deterministic comb, is given by

$$F := F^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} \otimes \frac{I^{\mathcal{I}_2\mathcal{O}_2}}{d} \otimes \cdots \otimes \frac{I^{\mathcal{I}_d\mathcal{O}_d}}{d} \otimes \frac{I^{\mathcal{O}_0}}{d} \tag{C.27}$$

where

$$F^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} := \frac{I^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1}}{d} - \varepsilon S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} \tag{C.28}$$

$$= \frac{I^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1}}{d} - \varepsilon\Bigg\{\frac{I^{\mathcal{I}_0}}{d_0} \otimes \mathrm{Tr}_{\mathcal{I}_0} S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} + \sum_{i=1}^{d_0^2-1}\sum_{j=1}^{d^2-1} \alpha_{ij} h_i^{\mathcal{I}_0} \otimes [g_j^{\mathcal{I}_1} \otimes I^{\mathcal{O}_1}]$$

$$+ \sum_{i=1}^{d_0^2-1}\sum_{j=1}^{d^2-1} \beta_{ij} h_i^{\mathcal{I}_0} \otimes [I^{\mathcal{I}_1} \otimes g_j^{\mathcal{O}_1}]\Bigg\}. \tag{C.29}$$

This F summed up with S satisfies the causal condition by construction, but it does not satisfy the neutralization condition Eq. (C.25). Thus, it is enough to construct $N \geq 0$ that satisfies the following conditions

$$\mathrm{Tr}_{\mathcal{O}_0} N - N^{(d)} \otimes \frac{I^{\mathcal{O}_d}}{d} = 0 \tag{C.30}$$

$$\mathrm{Tr}_{\mathcal{I}_k} N^{(k)} - N^{(k-1)} \otimes \frac{I^{\mathcal{O}_{k-1}}}{d} = 0 \quad (3 \leq k \leq d) \tag{C.31}$$

$$\mathrm{Tr}_{\mathcal{I}_2} N^{(2)} - N^{(1)} \otimes \frac{I^{\mathcal{O}_1}}{d} = d^{d-1}(F^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} - F^{\mathcal{I}_0\mathcal{I}_1} \otimes \frac{I^{\mathcal{O}_1}}{d}) \tag{C.32}$$

$$\mathrm{Tr}_{\mathcal{I}_1} N^{(1)} - (\mathrm{Tr} N)\frac{I^{\mathcal{I}_0}}{d_0} = 0 \tag{C.33}$$

$$\Pi_{sym}^{\mathcal{I}\mathcal{O}} N \Pi_{sym}^{\mathcal{I}\mathcal{O}} = \frac{J_{id}^{\mathcal{I}_0\mathcal{O}_0}}{d_0} \otimes \mathrm{Tr}_{\mathcal{I}_0\mathcal{O}_0}[\Pi_{sym}^{\mathcal{I}\mathcal{O}} N \Pi_{sym}^{\mathcal{I}\mathcal{O}}], \tag{C.34}$$

where $N^{(d)} := \mathrm{Tr}_{\mathcal{O}_d\mathcal{O}_0} N$ and $N^{(k-1)} := \mathrm{Tr}_{\mathcal{O}_{k-1}\mathcal{I}_k} N^{(k)}$ for $k = 2, \ldots, d$.

We divide the proof into two parts, by introducing the operator $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}} := \mathrm{Tr}_{\mathcal{O}_0} N$. In the first part of the proof, we show the existence of $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$, and the neutralization condition Eq. (C.34) is replaced by

$$\Pi_{sym}^{\mathcal{I}\mathcal{O}} N^{\mathcal{I}_0\mathcal{I}\mathcal{O}} \Pi_{sym}^{\mathcal{I}\mathcal{O}} = \frac{I^{\mathcal{I}_0}}{d_0} \otimes \mathrm{Tr}_{\mathcal{I}_0}[\Pi_{sym}^{\mathcal{I}\mathcal{O}} N^{\mathcal{I}_0\mathcal{I}\mathcal{O}} \Pi_{sym}^{\mathcal{I}\mathcal{O}}]. \tag{C.35}$$

In the second part of the proof (Lemma C.4), we construct the desired N from $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$. In both constructions, the following three conditions are considered: the positivity, the causal condition, and the neutralization condition.

(First part: construction of $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$) Let $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$ be

$$
\begin{aligned}
N^{\mathcal{I}_0\mathcal{I}\mathcal{O}} := & \frac{1}{d} I^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} \otimes \frac{I^{\mathcal{I}_2\mathcal{O}_2}}{d} \otimes \cdots \otimes \frac{I^{\mathcal{I}_d\mathcal{O}_d}}{d} \\
& - \varepsilon \Bigg\{ \frac{I^{\mathcal{I}_0}}{d_0} \otimes \mathrm{Tr}_{\mathcal{I}_0} S_t^{\mathcal{I}_0\mathcal{I}_1\mathcal{O}_1} \otimes \frac{I^{\mathcal{I}_2\mathcal{O}_2}}{d} \otimes \cdots \otimes \frac{I^{\mathcal{I}_d\mathcal{O}_d}}{d} \\
& + \sum_{i,j\geq 1} \alpha_{ij} h_i^{\mathcal{I}_0} \otimes [g_j^{\mathcal{I}_1} \otimes I^{\mathcal{O}_1}] \otimes \frac{I^{\mathcal{I}_2\mathcal{O}_2}}{d} \otimes \cdots \otimes \frac{I^{\mathcal{I}_d\mathcal{O}_d}}{d} \\
& + \sum_{i,j\geq 1} (-\alpha_{ij}) h_i^{\mathcal{I}_0} \otimes \frac{I^{\mathcal{I}_1\mathcal{O}_1}}{d} \otimes [g_j^{\mathcal{I}_2} \otimes I^{\mathcal{O}_2}] \otimes \cdots \otimes \frac{I^{\mathcal{I}_d\mathcal{O}_d}}{d} \\
& + \sum_{i,j\geq 1} \beta_{ij} h_i^{\mathcal{I}_0} \otimes [I^{\mathcal{I}_1} \otimes g_j^{\mathcal{O}_1}] \otimes \frac{I^{\mathcal{I}_2\mathcal{O}_2}}{d} \otimes \cdots \otimes \frac{I^{\mathcal{I}_d\mathcal{O}_d}}{d} \\
& + \sum_{i,j\geq 1,\vec{k_2}} \beta_{ij} a_{2,\vec{k_2}} h_i^{\mathcal{I}_0} \otimes [g_{k_{2,1}}^{\mathcal{I}_1} \otimes g_j^{\mathcal{O}_1}] \otimes [g_{k_{2,2}}^{\mathcal{I}_2} \otimes \frac{I^{\mathcal{O}_2}}{d}] \otimes \frac{I^{\mathcal{I}_3\mathcal{O}_3}}{d} \cdots \otimes \frac{I^{\mathcal{I}_d\mathcal{O}_d}}{d} \\
& + \cdots + \\
& + \sum_{i,j\geq 1,\vec{k_d}} \beta_{ij} a_{d,\vec{k_d}} h_i^{\mathcal{I}_0} \otimes [g_{k_{d,1}}^{\mathcal{I}_1} \otimes g_j^{\mathcal{O}_1}] \otimes [g_{k_{d,2}}^{\mathcal{I}_2} \otimes \frac{I^{\mathcal{O}_2}}{d}] \otimes \cdots \otimes [g_{k_{d,d}}^{\mathcal{I}_d} \otimes \frac{I^{\mathcal{O}_d}}{d}] \Bigg\},
\end{aligned}
\tag{C.36}
$$

where the summation on $\vec{k_m} = (k_{m,1}, k_{m,2}, \ldots, k_{m,m})$ denotes the summation on $\{k_{i,j} = 0, \ldots, d^2 - 1\}$ for each term, and coefficients $a_{m,\vec{k_m}}$ are determined in the following.

(Positivity) The positivity of $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$ is trivial for small enough ε. That is, since $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$ is of the form $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}} = I/d^d + \varepsilon N'$ where N' does not depend on ε, there exists $\varepsilon > 0$ such that $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$ is strictly positive.

(Causal condition) Here we show that the causal conditions Eqs. (C.30)-(C.33) are satisfied. We first remark that the 1st, 2nd, 3rd and 5th lines sum up to F, and we can write $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$ as $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}} = F + F'_s + \sum_{m=2}^d F'_m$ where F'_s corresponds to the 4th line, and $F'_2, \ldots, F'_d$ correspond to the 6th to the last line. Then it is enough to show that all $F' \in \{F'_i\}_{i=s,2,3,\ldots,d}$ satisfies

$$\mathrm{Tr}_{\mathcal{O}_0} F' - F'^{(d)} \otimes \frac{I^{\mathcal{O}_d}}{d} = 0 \tag{C.37}$$

$$\mathrm{Tr}_{\mathcal{I}_k} F'^{(k)} - F'^{(k-1)} \otimes \frac{I^{\mathcal{O}_{k-1}}}{d} = 0 \quad (2 \leq k \leq d) \tag{C.38}$$

$$\mathrm{Tr}_{\mathcal{I}_1} F'^{(1)} - (\mathrm{Tr} F') \frac{I^{\mathcal{I}_0}}{d_0} = 0, \tag{C.39}$$

where $F'^{(d)} := \mathrm{Tr}_{\mathcal{O}_d\mathcal{O}_0} F'$ and $F'^{(k-1)} := \mathrm{Tr}_{\mathcal{O}_{k-1}\mathcal{I}_k} F'^{(k)}$ for $k = 2, \ldots, d$.

It is trivial that Eq. (C.37) is satisfied for all F'. It is also trivial to see that Eqs. (C.38),(C.39) are satisfied for F'_a. Thus, we consider Eqs. (C.38),(C.39) for $F'_2, \dots, F'_d$. We can see that the l.h.s. of these equations are always of the form $\mathrm{Tr}_{\mathcal{I}_k \cdots}(F' - \mathrm{Tr}_{\mathcal{O}_{k-1}} F' \otimes \frac{I^{\mathcal{I}_{k-1}}}{d})$, and F'_m satisfies these conditions when $m < k$ because F'_m already has the term $\frac{I^{\mathcal{I}_k}}{d}$. In order to satisfy these conditions for $m \geq k$, we assume that the coefficients $a_{m,\vec{k_m}}$ satisfy

$$a_{m,\vec{k_m}} := a_{m,k_{m,1},k_{m,2},\dots,k_{m,m}} = 0 \quad \text{for} \quad k_{m,m} = 0, \tag{C.40}$$

which is compatible with the following arguments on the neutralization condition. By choosing these coefficients, $\mathrm{Tr}_{\mathcal{I}_k \cdots} F'_m = 0$ is satisfied and Eqs. (C.38),(C.39) are also satisfied.

(Neutralization condition) Now we present a construction of coefficients $a_{m,\vec{k_m}}$ such that Eq. (C.35) is satisfied. This condition is satisfied independently for the 1st line, 2nd line, the sum of 3rd and 4th lines, and the sum of the rest. First of all, it is trivial that the 1st line and the 2nd line satisfy the condition, as they have $I^{\mathcal{I}_0}$ in the system $\mathcal{I}_0$. The sum of the 3rd and 4th lines vanishes on $\Pi_{sym}^{\mathcal{IO}}$, i.e. satisfies the condition with the r.h.s. being 0, because $\Pi_{sym}^{\mathcal{IO}} P_\sigma M P_\sigma \Pi_{sym}^{\mathcal{IO}} = \Pi_{sym}^{\mathcal{IO}} M \Pi_{sym}^{\mathcal{IO}}$ holds for any permutation σ and an arbitrary operator M. For the sum of 5th line and after, we see that for each $i, j \geq 1$, it can be written as $\beta_{ij} h_i^{\mathcal{I}_0} \otimes C_j$ with

$$\begin{aligned}
C_j &= [I^{\mathcal{I}_1} \otimes g_j^{\mathcal{O}_1}] \otimes \frac{I^{\mathcal{I}_2\mathcal{O}_2}}{d} \otimes \cdots \otimes \frac{I^{\mathcal{I}_d\mathcal{O}_d}}{d} \\
&+ \sum_{\vec{k_2}} a_{2,\vec{k_2}} [g_{k_{2,1}}^{\mathcal{I}_1} \otimes g_j^{\mathcal{O}_1}] \otimes [g_{k_{2,2}}^{\mathcal{I}_2} \otimes \frac{I^{\mathcal{O}_2}}{d}] \otimes \frac{I^{\mathcal{I}_3\mathcal{O}_3}}{d} \cdots \otimes \frac{I^{\mathcal{I}_d\mathcal{O}_d}}{d} \\
&+ \cdots + \\
&+ \sum_{\vec{k_d}} a_{d,\vec{k_d}} [g_{k_{d,1}}^{\mathcal{I}_1} \otimes g_j^{\mathcal{O}_1}] \otimes [g_{k_{d,2}}^{\mathcal{I}_2} \otimes \frac{I^{\mathcal{O}_2}}{d}] \otimes \cdots \otimes [g_{k_{d,d}}^{\mathcal{I}_d} \otimes \frac{I^{\mathcal{O}_d}}{d}]
\end{aligned} \tag{C.41}$$

$$\begin{aligned}
&= [I^{\mathcal{I}_1} \otimes I^{\mathcal{I}_2} \otimes \cdots \otimes I^{\mathcal{I}_d} + \sum_{\vec{k_2}} a_{2,\vec{k_2}} g_{k_{2,1}}^{\mathcal{I}_1} \otimes g_{k_{2,2}}^{\mathcal{I}_2} \otimes I^{\mathcal{I}_3} \otimes \cdots \otimes I^{\mathcal{I}_d} \\
&\quad + \cdots + \sum_{\vec{k_d}} a_{d,\vec{k_d}} g_{k_{d,1}}^{\mathcal{I}_1} \otimes g_{k_{d,2}}^{\mathcal{I}_2} \otimes g_{k_{d,3}}^{\mathcal{I}_3} \otimes \cdots \otimes g_{k_{d,d}}^{\mathcal{I}_d}] \\
&\otimes [g_j^{\mathcal{O}_1} \otimes \frac{I^{\mathcal{O}_2}}{d} \otimes \cdots \otimes \frac{I^{\mathcal{O}_d}}{d}].
\end{aligned} \tag{C.42}$$

In the following, we show that the neutralization condition is satisfied for each i, j, by showing that C_j vanishes on $\Pi_{sym}^{\mathcal{IO}}$ as $\Pi_{sym}^{\mathcal{IO}} C_j \Pi_{sym}^{\mathcal{IO}} = 0$.

Here, we choose the coefficients $\{a_{m,\vec{k_m}}\}$ such that the first term is the d qudit (unnormalized) totally antisymmetric state $d^d A_d = d^d |A_d\rangle\langle A_d|$. Such coefficients are available as follows. Note that we assumed Eq. (C.40) in the causal condition part. Since $g_{i_1} \otimes g_{i_2} \otimes \cdots g_{i_d}$ forms a basis, any operator including A_d can be written as $\sum_{i_1,i_2,\ldots,i_d} a_{i_1,i_2,\ldots,i_d} g_{i_1} \otimes g_{i_2} \otimes \cdots \otimes g_{i_d}$. However, the coefficients $\{a_{m,\vec{k_m}}\}$ have the constraint given by Eq. (C.40) and cannot cover arbitrary operators. Especially, it lacks the terms $g_{i_1} \otimes I \otimes \cdots \otimes I$ with $i_1 \neq 0$. The totally antisymmetric state satisfies $\mathrm{Tr}_{2,\ldots,d} A_d = I_1$, and the coefficients corresponding to these terms that containing only one traceless operator g_{i_1} are actually 0. Thus, there exists a set of $\{a_{m,\vec{k_m}}\}$ satisfying Eq. (C.40) and that Eq. (C.42) can be evaluated as

$$C_j = d^d A_d^{\mathcal{I}} \otimes [g_j^{\mathcal{O}_1} \otimes \frac{I^{\mathcal{O}_2}}{d} \otimes \cdots \otimes \frac{I^{\mathcal{O}_d}}{d}] =: d A_d^{\mathcal{I}} \otimes M_j^{\mathcal{O}}. \tag{C.43}$$

Now we show that C_j vanishes on $\Pi_{sym}^{\mathcal{IO}}$. Consider that $\Pi_{sym}^{\mathcal{IO}} = \sum_\sigma P_\sigma^{\mathcal{IO}} = \sum_\sigma P_\sigma^{\mathcal{I}} \otimes P_\sigma^{\mathcal{O}}$ and $P_\sigma^{\mathcal{I}} |A_d\rangle = sgn(\sigma) |A_d\rangle$, $\Pi_{sym}^{\mathcal{IO}} (A_d^{\mathcal{I}} \otimes M_j^{\mathcal{O}}) \Pi_{sym}^{\mathcal{IO}}$ can be evaluated as

$$\Pi_{sym}^{\mathcal{IO}} (A_d^{\mathcal{I}} \otimes M_j^{\mathcal{O}}) \Pi_{sym}^{\mathcal{IO}} = A_d^{\mathcal{I}} \otimes [\sum_\sigma sgn(\sigma) P_\sigma^{\mathcal{O}}] M_j^{\mathcal{O}} [\sum_{\sigma'} sgn(\sigma') P_{\sigma'}^{\mathcal{O}}] \tag{C.44}$$

$$= A_d^{\mathcal{I}} \otimes A_d^{\mathcal{O}} M_j^{\mathcal{O}} A_d^{\mathcal{O}} \tag{C.45}$$

Also, the equation

$$\mathrm{Tr}\, A_d^{\mathcal{O}} M_j^{\mathcal{O}} A_d^{\mathcal{O}} = \langle A_d | g_j^{\mathcal{O}_1} \otimes I^{\mathcal{O}_2} \otimes \cdots \otimes I^{\mathcal{O}_d} | A_d \rangle \tag{C.46}$$

$$= \mathrm{Tr}\, g_j^{\mathcal{O}_1} = 0 \tag{C.47}$$

holds because $g_j^{\mathcal{O}_1}$ are traceless for $j \geq 1$. Thus, we obtain $A_d^{\mathcal{O}} M_j^{\mathcal{O}} A_d^{\mathcal{O}} = 0$ and $\Pi_{sym}^{\mathcal{IO}} C_j \Pi_{sym}^{\mathcal{IO}} = 0$ for $j \geq 1$.

(Second part: construction of N from $N^{\mathcal{I}_0 \mathcal{IO}}$) We apply Lemma C.4 shown below. The operator $d^d N^{\mathcal{I}_0 \mathcal{IO}} = I + \varepsilon N'$ corresponds to $M^{AB} = I + \varepsilon M'$, $d^{d+1} N$ corresponds to M^{ABC}, and systems A, B, C correspond to $\mathcal{I}_0, \mathcal{I} \otimes \mathcal{O}, \mathcal{O}_0$ respectively.

□

Lemma C.4. *Let $\mathcal{H}_A, \mathcal{H}_B, \mathcal{H}_C \simeq \mathcal{H}_A$ be Hilbert spaces with dimensions d_0, d_B, d_0, Π^B be a projector on $\mathcal{L}(\mathcal{H}_B)$, and $J_{id}^{AC} = d_0 \phi^+$ be the maximally entangled state on $\mathcal{H}_A \otimes \mathcal{H}_C$. Given an operator $M' \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$, there exists $\varepsilon > 0$ such that the following holds. If $M^{AB} = I + \varepsilon M'$ satisfies*

$$M^{AB} \geq 0 \tag{C.48}$$

$$\Pi^B M^{AB} \Pi^B = \frac{I^A}{d_0} \otimes \mathrm{Tr}_A \Pi^B M^{AB} \Pi^B, \tag{C.49}$$

there exists an operator $M^{ABC} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C)$ *satisfying*

$$M^{ABC} \geq 0 \tag{C.50}$$

$$\mathrm{Tr}_C M^{ABC} = M^{AB} \tag{C.51}$$

$$\Pi^B M^{ABC} \Pi^B = \frac{1}{d_0} J_{id}^{AC} \otimes \mathrm{Tr}_{AC} \Pi^B M^{ABC} \Pi^B. \tag{C.52}$$

Proof. Let $\{h_i\}$ with $h_0 = I$ be a Hermitian basis for $\mathcal{H}_A$ and $\mathcal{H}_C$. Let $M_i^B := \frac{1}{d_0} \mathrm{Tr}_A h_i^A M^{AB}$, so that $M^{AB} = \sum_i h_i^A \otimes M_i^B$ holds. Note that with this decomposition, the condition Eq. (C.49) is given by $\Pi^B M^{AB} \Pi^B = I^A \otimes \Pi^B M_0^B \Pi^B$ and $\Pi^B M_i^B \Pi^B = 0$ for $i \neq 0$.

For simplicity of the proof, we give a construction of M^{ABC} first as

$$\begin{aligned} M^{ABC} := {} & J_{id}^{AC} \otimes \Pi^B M_0^B \Pi^B + \frac{1}{d_0} (I^A \otimes I^C) \otimes \Pi_\perp^B M_0^B \Pi_\perp^B \\ & + \frac{1}{d_0} \sum_{i \geq 1} h_i^A \otimes \Pi_\perp^B M_i^B \Pi_\perp^B \otimes I^C \\ & + \frac{1}{d_0} \sum_{k \geq 0} (h_k^A \otimes I^C + \sum_{i \geq 0, j \geq 1} \alpha_{ijk} h_i^A \otimes h_j^C) \otimes \Pi^B M_k^B \Pi_\perp^B \\ & + \frac{1}{d_0} \sum_{k \geq 0} (h_k^A \otimes I^C + \sum_{i \geq 0, j \geq 1} \alpha_{ijk}^* h_i^A \otimes h_j^C) \otimes \Pi_\perp^B M_k^B \Pi^B, \end{aligned} \tag{C.53}$$

where $\{\alpha_{ijk}\}$ are complex numbers determined in the following. It is easy to see that the causal condition Eq. (C.51) and the neutralization condition Eq. (C.52) are satisfied, and the remaining condition for M^{ABC} is the positivity.

In order to guarantee the positivity, we first consider the support given by the projector

$$\Pi_{sup} = (\phi^+)^{AC} \otimes \Pi^B + I^{AC} \otimes \Pi_\perp^B \tag{C.54}$$

with the projector $\phi^+ = J_{id}/d_0$, then obtain parameters $\{\alpha_{ijk}\}$ so that M^{ABC} is on this support, and finally show that M^{ABC} is positive with small enough ε. The condition $\Pi_{sup} M^{ABC} \Pi_{sup} = M^{ABC}$ is satisfied if the following equality holds

$$(\phi^+)^{AC} (h_k^A \otimes I^C + \sum_{i \geq 0, j \geq 1} \alpha_{ijk} h_i^A \otimes h_j^C) I^{AC} = (h_k^A \otimes I^C + \sum_{i \geq 0, j \geq 1} \alpha_{ijk} h_i^A \otimes h_j^C), \tag{C.55}$$

or equivalently

$$\phi^+ A_k = A_k \tag{C.56}$$

with $A_k := h_k^A \otimes I^C + \sum_{i\geq 0, j\geq 1} \alpha_{ijk} h_i^A \otimes h_j^C$. Since $\{\alpha_{ijk}\}$ can be any complex numbers, the restrictions for $\{A_k\}$ are given by

$$\mathrm{Tr}(h_{k'} \otimes I) A_k = d_0^2 \delta_{kk'} \tag{C.57}$$

for all k, k'. In order to satisfy $\phi^+ A_k = A_k$, A_k should be decomposed as $A_k = |\phi^+\rangle\langle a_k|$, where $|a_k\rangle$ is an unnormalized vector. Let $|a_k\rangle = \sum_{m,n=0}^{d_0-1} a_{mn}^{(k)} |mn\rangle$, then the condition for $a_{mn}^{(k)}$ is that

$$\mathrm{Tr}(h_{k'} \otimes I) A_k = \sum_{m,n=0}^{d_0-1} (a_{mn}^{(k)})^* \langle m|h_{k'}|n\rangle = d_0^2 \delta_{kk'}, \tag{C.58}$$

for $k, k' = 0, \ldots, d_0^2 - 1$. Here, the d_0^2 parameters a_{mn} can be chosen freely, and there are d_0^2 linear (and independent due to the orthogonality of $h_{k'}$) constraints, thus, there exists a feasible a_{mn}, A_k, and α_{ijk}. Therefore, $\Pi_{sup} M^{ABC} \Pi_{sup} = M^{ABC}$ holds.

For $M^{AB} = I$, a possible M^{ABC} is given by

$$M^{ABC} = J_{id}^{AC} \otimes \Pi^B + \frac{1}{d_0} I^{AC} \otimes \Pi_\perp^B =: M_0^{ABC}. \tag{C.59}$$

For $M^{AB} = I + \varepsilon M'$, the corresponding M^{ABC} can be written as

$$M^{ABC} = M_0^{ABC} + \varepsilon M'', \tag{C.60}$$

where M'' is an operator only depends on M', because the construction of M^{ABC} given by Eq. (C.53) is linear in M^{AB}. The non-zero minimum eigenvalue is given by

$$\min_{|\psi\rangle \in \Pi_{sup}} \langle\psi|M^{ABC}|\psi\rangle = \min_{|\psi\rangle \in \Pi_{sup}} [\langle\psi|M_0^{ABC}|\psi\rangle + \varepsilon \langle\psi|M''|\psi\rangle], \tag{C.61}$$

since $\Pi_{sup} M^{ABC} \Pi_{sup} = M^{ABC}$ is satisfied. The minimum eigenvalue on the support Π_{sup} is given by minimizing the $|\psi\rangle$ with vectors only on Π_{sup}, in which case the first term is strictly positive, especially larger than $1/d_0$. Thus, there exists $\varepsilon > 0$ such that the minimum eigenvalue on Π_{sup} is greater than 0, and the positivity of M^{ABC} is guaranteed.

□

Remark C.1. In the second part for the proof of Theorem C.1 (mostly equivalent to Lemma C.4), the condition Eq. (C.30) (Eq. (C.51)) is assumed which corresponds to the causal condition that the corresponding Choi operator is a sequential supemap or quantum comb. However, when the indefinite causal order is allowed, this causal condition can be relaxed and the construction of N

from $N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$ can be replaced as follows instead of Lemma C.4. The conditions for an indefinite causal order supermap are that the corresponding Choi operator is positive, and that when the input operations are CPTP maps, the output operation is also a CPTP map. Here we consider a subset of such supermaps of which Choi operators satisfy the following condition:

$$\mathrm{Tr}_{\mathcal{O}_0} C = \sum_\sigma p_\sigma C_\sigma^{\mathcal{I}_0\mathcal{I}\mathcal{O}} \tag{C.62}$$

where p_σ are probabilities summing up to 1, and $C_\sigma^{\mathcal{I}_0\mathcal{I}\mathcal{O}}$ denotes a sequential supermap where the order of input operations are permuted with respect to the permutation σ. This is a strictly stronger condition than that of general indefinite causal order supermaps, but many quantum supermaps satisfy this condition such as quantum switch.

Let $N_\sigma^{\mathcal{I}_0\mathcal{I}\mathcal{O}} := P_\sigma^{\mathcal{I}\mathcal{O}}(N^{\mathcal{I}_0\mathcal{I}\mathcal{O}})P_\sigma^{\mathcal{I}\mathcal{O}}$ be the probabilistic comb with the order of input operations permuted by σ. We define N as

$$N := (\frac{1}{N!}\sum_\sigma N_\sigma^{\mathcal{I}_0\mathcal{I}\mathcal{O}}) \otimes \frac{I^{\mathcal{O}_0}}{d_0} + \frac{1}{d_0}\sum_{ij\geq 1}\eta_{ij} h_i^{\mathcal{I}_0}\Pi_{sym}^{\mathcal{I}\mathcal{O}}(\frac{1}{N!}\sum_\sigma N_\sigma^{\mathcal{I}_0\mathcal{I}\mathcal{O}})\Pi_{sym}^{\mathcal{I}\mathcal{O}} \otimes h_j^{\mathcal{O}_0} \tag{C.63}$$

$$= \frac{I^{\mathcal{I}_0}}{d_0} \otimes \frac{1}{N!}\sum_\sigma (\mathrm{Tr}_{\mathcal{I}_0}\Pi_{sym}^{\mathcal{I}\mathcal{O}} N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}\Pi_{sym}^{\mathcal{I}\mathcal{O}}) \otimes \frac{I^{\mathcal{O}_0}}{d_0} + \frac{1}{N!}\sum_\sigma \Pi_{sym}^{\perp}(N^{\mathcal{I}_0\mathcal{I}\mathcal{O}})\Pi_{sym}^{\perp} \otimes \frac{I^{\mathcal{O}_0}}{d_0}$$

$$+ \sum_{ij\geq 1}\eta_{ij}\frac{h_i^{\mathcal{I}_0}}{d_0} \otimes \frac{1}{N!}\sum_\sigma (\mathrm{Tr}_{\mathcal{I}_0}\Pi_{sym}^{\mathcal{I}\mathcal{O}} N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}\Pi_{sym}^{\mathcal{I}\mathcal{O}}) \otimes \frac{h_j^{\mathcal{O}_0}}{d_0} \tag{C.64}$$

$$= \frac{1}{d_0}J_{id}^{\mathcal{I}_0\mathcal{O}_0} \otimes \frac{1}{N!}\sum_\sigma (\mathrm{Tr}_{\mathcal{I}_0}\Pi_{sym}^{\mathcal{I}\mathcal{O}} N^{\mathcal{I}_0\mathcal{I}\mathcal{O}}\Pi_{sym}^{\mathcal{I}\mathcal{O}}) + \frac{1}{N!}\sum_\sigma \Pi_{sym}^{\perp}(N^{\mathcal{I}_0\mathcal{I}\mathcal{O}})\Pi_{sym}^{\perp} \otimes \frac{I^{\mathcal{O}_0}}{d_0} \tag{C.65}$$

where the coefficients η_{ij} are determined by $J_{id} = \frac{1}{d_0} I \otimes I + \frac{1}{d_0}\sum_{ij\geq 1}\eta_{ij} h_i \otimes h_j$. In the first equality, we also use the fact that if an operator is permutation invariant, it is block diagonal in $\Pi_{sym}^{\mathcal{I}\mathcal{O}}$ and $\Pi_{sym}^{\perp}$, that is, the off-diagonal terms vanishes as

$$\Pi_{sym}^{\mathcal{I}\mathcal{O}}(\frac{1}{N!}\sum_\sigma N_\sigma^{\mathcal{I}_0\mathcal{I}\mathcal{O}})\Pi_{sym}^{\perp} = \Pi_{sym}^{\mathcal{I}\mathcal{O}}(\frac{1}{N!}\sum_\sigma P_\sigma^{\mathcal{I}\mathcal{O}}(N^{\mathcal{I}_0\mathcal{I}\mathcal{O}})P_\sigma^{\mathcal{I}\mathcal{O}})(I - \Pi_{sym}^{\mathcal{I}\mathcal{O}}) \tag{C.66}$$

$$= \Pi_{sym}^{\mathcal{I}\mathcal{O}}\frac{1}{N!}\sum_\sigma (N^{\mathcal{I}_0\mathcal{I}\mathcal{O}})(P_\sigma^{\mathcal{I}\mathcal{O}} - \Pi_{sym}^{\mathcal{I}\mathcal{O}}) \tag{C.67}$$

$$= \Pi_{sym}^{\mathcal{I}\mathcal{O}}(N^{\mathcal{I}_0\mathcal{I}\mathcal{O}})(\Pi_{sym}^{\mathcal{I}\mathcal{O}} - \Pi_{sym}^{\mathcal{I}\mathcal{O}}) = 0. \tag{C.68}$$

By this construction, the positivity of N is preserved because both terms in Eq. (C.63) are positive, and the neutralization condition $\Pi_{sym}^{\mathcal{I}\mathcal{O}} N \Pi_{sym}^{\mathcal{I}\mathcal{O}} = J_{id}/d_0 \otimes$

$\mathrm{Tr}_{\mathcal{I}_0\mathcal{O}_0}\Pi_{sym}^{\mathcal{IO}}N\Pi_{sym}^{\mathcal{IO}}$ is also satisfied. To see the causal condition can be satisfied, we first note that

$$\mathrm{Tr}_{\mathcal{O}_0}N = \frac{1}{N!}\sum_{\sigma} N_{\sigma}^{\mathcal{I}_0\mathcal{IO}} \tag{C.69}$$

holds. Since there exists an operator S such that $\mathrm{Tr}_{\mathcal{O}_0}(S+N)$ satisfies the sequential condition (which is actually given by Eq. (C.26)), by defining $S_{\sigma}^{\mathcal{I}_0\mathcal{IO}} := P_{\sigma}^{\mathcal{IO}}(\mathrm{Tr}_{\mathcal{O}_0}S)P_{\sigma}^{\mathcal{IO}}$, $C_{\sigma}^{\mathcal{I}_0\mathcal{IO}} := S_{\sigma}^{\mathcal{I}_0\mathcal{IO}} + N_{\sigma}^{\mathcal{I}_0\mathcal{IO}}$ and $p_{\sigma} = 1/N!$, we can see that the causal condition Eq. (C.62) is satisfied.

Appendix D

Impossibility of Success-or-Draw for Unitary Inversion with a Single Input Operation

For the two-dimensional unitary inversion, we show that it is not possible to have a success-or-draw structure if we have only a single use of the input unitary operation. Especially, we show the only solution to the following SDP is $p = 0$. Note that we denote $d = 2$ in order to clarify that it corresponds to the dimension.

$$\max \quad p \tag{D.1}$$

$$\text{s.t.} \quad \mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1}[S {J_U}^T] = pJ_{U^{-1}} \tag{D.2}$$

$$\mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1}[N {J_U}^T] \leq dJ_{id} \tag{D.3}$$

$$S \geq 0, N \geq 0 \tag{D.4}$$

$$\mathrm{Tr}_{\mathcal{O}_0}(S+N) = \mathrm{Tr}_{\mathcal{O}_1\mathcal{O}_0}(S+N) \otimes \frac{I^{\mathcal{O}_1}}{d} \tag{D.5}$$

$$\mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1\mathcal{O}_0}(S+N) = \mathrm{Tr}(S+N)\frac{I^{\mathcal{I}_0}}{d} \tag{D.6}$$

Proof. Assuming that $\{p, S, N\}$ is a solution to this SDP, then for any U, $\{p, (U^{\mathcal{I}_1} \otimes U^{\mathcal{O}_0})S(U^{\mathcal{I}_1} \otimes U^{\mathcal{O}_0}), U^{\mathcal{I}_1} N U^{\mathcal{I}_1}\}$ is also a solution to this SDP, because it satisfies all of the conditions. By defining $S' = \int dU (U^{\mathcal{I}_1} \otimes U^{\mathcal{O}_0})S(U^{\mathcal{I}_1} \otimes U^{\mathcal{O}_0})$ and $N' = \int dU U^{\mathcal{I}_1} N U^{\mathcal{I}_1}$, we obtain $\{p, S', N'\}$ which is also a solution to this SDP. Thus, without loss of generality, we can assume the following commutation relation

$$[S, U^{\mathcal{I}_1} \otimes U^{\mathcal{O}_0}] = 0, \tag{D.7}$$

$$[N, U^{\mathcal{I}_1}] = 0. \tag{D.8}$$

From the second commutation relation Eq.(D.8) and Schur's lemma, N can be decomposed as

$$N = N^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0} \otimes \frac{I^{\mathcal{I}_1}}{d}. \tag{D.9}$$

Consider Eq. (D.3) with $U = I$, we obtain

$$dJ_{id} \geq \mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1}[(N^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0} \otimes \frac{I^{\mathcal{I}_1}}{d})J_{id}{}^T] \tag{D.10}$$

$$= \mathrm{Tr}_{\mathcal{O}_1}[N^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0}], \tag{D.11}$$

and $N^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0}$ can be decomposed as

$$N^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0} = N^{\mathcal{O}_1} \otimes J_{id}^{\mathcal{I}_0\mathcal{O}_0}/d \tag{D.12}$$

as follows. Let $N^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0} = \sum_i p_i |n_i^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0}\rangle\langle n_i^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0}|$. Since J_{id} is rank-1, Eq. (D.11) indicates that $\mathrm{Tr}_{\mathcal{O}_1}|n_i^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0}\rangle\langle n_i^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0}| \propto J_{id}$ holds for all i. Consider the Schmidt decomposition $|n_i^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0}\rangle = \sum_j \alpha_{ij}|a_j^{\mathcal{I}_0\mathcal{O}_0}\rangle \otimes |b_j^{\mathcal{O}_1}\rangle$, then $\mathrm{Tr}_{\mathcal{O}_1}|n_i^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0}\rangle\langle n_i^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0}| = \sum_j |\alpha_{ij}|^2 |a_j^{\mathcal{I}_0\mathcal{O}_0}\rangle\langle a_j^{\mathcal{I}_0\mathcal{O}_0}|$ is proportional to the rank-1 operator J_{id}, which means the only possible solution is that $|n_i^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0}\rangle = |(\phi^+)^{\mathcal{I}_0\mathcal{O}_0}\rangle \otimes |b_j^{\mathcal{O}_1}\rangle$ where $|\phi^+\rangle\langle\phi^+| = J_{id}/d$ is the maximally entangled state. Thus, $N^{\mathcal{I}_0\mathcal{O}_1\mathcal{O}_0}$ can be decomposed as Eq. (D.12).

On the other hand, we can show

$$S = pJ_Y^{\mathcal{I}_0\mathcal{O}_1} \otimes J_Y^{\mathcal{I}_1\mathcal{O}_0} \tag{D.13}$$

as follows. Note that $J_Y = d\psi^- = d|\psi^-\rangle\langle\psi^-|$ where $|\psi^-\rangle = (1/\sqrt{2})(|01\rangle - |10\rangle)$ is a maximally entangled state also known as the singlet state. From Eq.(D.7) and Schur's lemma, S can be decomposed as $S = S^{\mathcal{I}_0\mathcal{O}_1} \otimes J_Y^{\mathcal{I}_1\mathcal{O}_0}/d$. Let $S^{\mathcal{I}_0\mathcal{O}_1} = \sum_i p_i |s_i^{\mathcal{I}_0\mathcal{O}_1}\rangle\langle s_i^{\mathcal{I}_0\mathcal{O}_1}|$ and consider Eq. (D.2). Since the r.h.s. of Eq. (D.2) is rank-1, it is necessary for every i that

$$\mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1}[(|s_i^{\mathcal{I}_0\mathcal{O}_1}\rangle\langle s_i^{\mathcal{I}_0\mathcal{O}_1}| \otimes \frac{J_Y^{\mathcal{I}_1\mathcal{O}_0}}{d})J_{id}] \propto J_{id} \tag{D.14}$$

holds, where we choose $U = I$ in Eq. (D.2). Consider the Schmidt decomposition $|s_i^{\mathcal{I}_0\mathcal{O}_1}\rangle = \sum_j \alpha_{ij}|a_j\rangle^{\mathcal{I}_0} \otimes Y|b_j\rangle^{\mathcal{O}_1}$, where $\{|a_j\rangle\}$ and $\{|b_j\rangle\}$ are some basis and the Pauli operator Y is added for convenience. Then Eq. (D.14) become

$$\sum_j \alpha_{ij}|a_j\rangle^{\mathcal{I}_0} \otimes |b_j\rangle^{\mathcal{O}_0} \propto |\phi^+\rangle^{\mathcal{I}_0\mathcal{O}_0}. \tag{D.15}$$

and thus $|s_i^{\mathcal{I}_0\mathcal{O}_1}\rangle\langle s_i^{\mathcal{I}_0\mathcal{O}_1}|$ is proportional to J_Y. The constant factor is obtained by direct calculation, and Eq. (D.13) is proved.

By using the causal conditions, we obtain

$$\mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_0}(S+N) = \mathrm{Tr}_{\mathcal{I}_1\mathcal{O}_1\mathcal{O}_0}(S+N) \otimes \frac{I^{\mathcal{O}_1}}{d} = \mathrm{Tr}(S+N)\frac{I^{\mathcal{I}_0} \otimes I^{\mathcal{O}_1}}{d^2} = I^{\mathcal{I}_0} \otimes I^{\mathcal{O}_1} \tag{D.16}$$

and since S is given by Eq. (D.13), we obtain

$$N^{\mathcal{I}_0\mathcal{O}_1} = I^{\mathcal{I}_0\mathcal{O}_1} - pdJ_Y^{\mathcal{I}_0\mathcal{O}_1}. \tag{D.17}$$

On the other hand, Eq. (D.12) indicates $N^{\mathcal{I}_0\mathcal{O}_1} = N^{\mathcal{O}_1} \otimes I^{\mathcal{I}_0}/d$, and the only possible solution with Eq. (D.17) is $p = 0$.

□

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