

# Categorical Quantum Circuits

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This article takes large steps to connect two fields: the mathematical ideas appearing in category theory and the state of the art in quantum information science. Specifically, we present an explicit representation of dagger compact closed categories in terms of an extended form of quantum circuit or quantum network diagrams. We map the graphical calculus of the categories used in the axiomatization of Hilbert space quantum mechanics onto quantum circuits, making a suitable extension of categorical quantum theory applicable to problems stated in the language of quantum information science. The circuit diagrams themselves now become morphisms in a category, making quantum circuits a special case of a much more general mathematical framework. This approach introduces a new set of tools which can be used to manipulate and simplify quantum networks in novel ways: this has further applications in applying category theory and related ideas from higher mathematics to tensor network simulation.

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## I. INTRODUCTION

This work aims to extend the diagrammatic methods commonly used with the widely studied and ubiquitous quantum circuit model (QCM). The quantum circuit model was put into its current form in the pioneering work by Yao [1] which built on several other notable results including those by Deutsch. It has remained largely unchanged from this original formulation up to the present day, with perhaps the first exception being due to the early work by Aharonov, Kitaev and Nisan [2] who, in their formulation, replace pure states with state operators and unitary gates with completely positive maps. This overcomes several limitations of the standard QCM: such as representing measurements in the middle of the computation, decoherence, and probabilistic subroutines. The state of the art in graphical languages in use in quantum information science can be found in e.g. [3] where we note the early work in [4].

Diagrammatic methods in physics and in quantum information science have a long history [5–7]. Building on the results of reversible logic and computation, perhaps the first to note their importance in quantum information science was David Deutsch. The importance of diagrammatic methods stems from the fact that they enable one to perform mathematical reasoning and even actual calculations using intuitive graphical objects instead of abstract mathematical entities. Modern quantum circuit diagrams (QCDs) are highly sophisticated tools, even though many of their features were developed in a largely ad hoc manner.

Our work approaches the problem of developing diagrammatic methods from the direction of category theory but also employs ideas of tensor network theory and related concepts. Category theory is often used as a unifying language for mathematics, and in more recent times to formulate physical theories [8, 9]. One of the strong points of the applied area of mathematics known as categorical modeling is that it comes equipped with a powerful and intuitive graphical language that can be proven to be fully equivalent to the corresponding algebraic notation. In this regard, sometimes one might hear the statement: “category theory formally justifies it’s absence”.

Category theory has only recently been used to model quantum mechanics [10]. Connecting categorical methods to the established area of quantum circuit theory is possible as category theory provides the exact arena of mathematics concerned with the diagrammatic reasoning present in the existing methods to manipulate quantum circuits. These *string diagrams* capture the mathematical properties of how maps (states and operators in the circuit model) can be composed. By considering the categorical description of the mathematics used in quantum mechanics, one essentially gets quantum circuits for free!

Traditional QCDs are graphs that are planar and directed acyclic. These are a subclass of the graphs one can construct in a compact closed category. One can go past this class by considering the symmetric, compact structure of the category. This amounts to adding in maps that are equivalent to Bell states ( $\sum_i |ii\rangle$ ) and Bell effects ( $\sum_i \langle ii|$ ): one can then arrive at the well known results surrounding channel state duality. In addition to this duality, categorical duality [10] comes with an intuitive graphical interpretation which we have used to manipulate quantum circuits in new ways. For instance, by temporarily dropping causality (e.g. directed temporal ordering) one can with relative ease perform very nontrivial operations on the diagrams and then convert them back into a standard, physically implementable quantum circuits.

The categorical model of quantum theory makes rigorous several diagrammatic notations, however its range of applicability has lacked and the approach currently relies on a reduced set of the operations and identities already present and well known in the traditional quantum circuit (and more generally, quantum network) model. On the other hand, the circuit model does not e.g. exploit some of the elegant mathematical ideas appearing in modern higher mathematics.

Both category theory and the quantum circuit model are well developed fields, backed by years of fundamental research and an increasing number of publications. As we have mentioned, the state of the art in graphical languages in current use in quantum information science can be found in e.g. [3] where we note the early work in [4]. As in the theory of tensor network states [3], the theory of categories allows one to study the mathematical structure formed by the composition of processes themselves (see for instance work on tensor network states [11]).

Our main focus in this article is to connect these two fields: the mathematical ideas appearing in category theory with the state of the art in quantum information science. By showing how the structure of a compact closed category can be represented in a quantum circuit, and by showing how quantum circuits can be transformed using methods from category theory we derive results useful to both areas.

## A. Background reading

This work attempts to be mostly self contained. For those interested in the string diagrams, Selinger’s “Survey of graphical languages for monoidal categories” offers an excellent starting place [12]. The mathematical insight behind using pictures to represent these and related networks dates back to Penrose and in quantum circuits, to Deutsch. The mathematics behind category theory is based largely on a completeness result (originally proved by Joyal and Street) about the kinds of string diagrams we consider here (and actually the Kelly-Laplaza-Selinger coherence result [12–14]).

We build on ideas across several fields. This includes the work by Lafont [15] which was aimed at providing an algebraic theory for classical Boolean circuits. Lafont’s work is related to the more recent work on proof theory by Guiraud [16]. By considering quantum protocols, Samson Abramsky and Bob Coecke provided a categorical framework which they later called “Categorical quantum mechanics” [10]. A good deal of work built on different aspects of their model. In particular, by considering quantum observables related by Hadamard transforms, Bob Coecke and Ross Duncan made progress towards a categorical model of quantum theory applicable to problems in quantum information and computation [17].

Recently several tutorials on the categories and corresponding diagrammatic calculus have been made available. These include the survey [8], the more specialized paper [18] and the light read [19].

## B. Example

States and observables themselves are typically not viewed in a way that emphasizes their compositional structure, giving a categorical model of quantum computation the prospect of providing new insights. To get a feeling for the types of insights possible, let us consider the following digression which will be made precise in the main text.

Consider two single-qubit operations: the identity operator  $\mathbb{1}$ , which is represented as a wire in a QCD, and the NOT operation, represented as an  $X$  on a wire. They are given by the linear maps  $\mathbb{1} := |0\rangle\langle 0| + |1\rangle\langle 1|$  and  $X := |0\rangle\langle 1| + |1\rangle\langle 0|$ , which take vectors from the one-qubit Hilbert space  $\mathcal{H}_2$  back into itself:

$$\mathcal{H}_2 \xrightarrow{X} \mathcal{H}_2 \quad \text{and} \quad \mathcal{H}_2 \xrightarrow{\mathbb{1}} \mathcal{H}_2. \quad (1)$$

Now let us consider the state  $|\Phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$ . It can be described as a map from the complex numbers into the Hilbert space of two qubits  $\mathcal{H}_2 \otimes \mathcal{H}_2$ , that is,

$$\mathbb{C} \xrightarrow{\Phi^+} \mathcal{H}_2 \otimes \mathcal{H}_2, \quad \Phi^+ : z \mapsto z|\Phi^+\rangle. \quad (2)$$

$\Phi^+(1) = |\Phi^+\rangle$  uniquely determines  $\Phi^+$  by linearity of the map.

What does one gain by thinking of quantum states like this? In the categorical approach, using compact structures one can derive canonical isomorphism between maps and states which will provide among other things an intuitive generalisation of the Choi-Jamiołkowski isomorphism (see Appendix D). We shall see that every map of *type*  $\mathcal{H}_2 \rightarrow \mathcal{H}_2$  gives rise to a map of type  $\mathbb{C} \rightarrow \mathcal{H}_2 \otimes \mathcal{H}_2$ , corresponding to a ket, and a map of type  $\mathcal{H}_2 \otimes \mathcal{H}_2 \rightarrow \mathbb{C}$ , corresponding to a bra. This is illustrated here using the identity map  $\mathbb{1}$ :<sup>1</sup>

$$\begin{aligned} \Phi^+ : \mathbb{C} \rightarrow \mathcal{H}_2 \otimes \mathcal{H}_2 &\cong \mathbb{1} : \mathcal{H}_2 \rightarrow \mathcal{H}_2 \cong \Phi^{+\dagger} : \mathcal{H}_2 \otimes \mathcal{H}_2 \rightarrow \mathbb{C} \\ |00\rangle + |11\rangle &\cong |0\rangle\langle 0| + |1\rangle\langle 1| \cong \langle 00| + \langle 11|. \end{aligned} \quad (3)$$

This amounts to being able to bend wires in quantum circuit diagrams.

## II. CATEGORIES

For the purpose of being self contained, we will sketch the basic definitions from category theory that surround the present work, in a way that we hope appeals to researchers working on quantum information

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<sup>1</sup> For a second one might wrongly suspect that the left hand side in Eq. (3) is the result of a partial trace, but we could have equally well illustrated this isomorphism with  $|000\rangle + |111\rangle \cong |00\rangle\langle 0| + |11\rangle\langle 1|$ .

theory. We will skim over details not essential to the present study. In particular, this will include several of the more technical points of these structures such as natural isomorphisms and coherence axioms. For a more complete treatment of the subject, see e.g. [12].

**Definition 1** (Category). A *category*  $\mathcal{C}$  is an algebraic structure that consists of

1.  $\text{ob}(\mathcal{C}) = \{A, B, C, \dots\}$ , a collection of *objects*.
2.  $\text{hom}(\mathcal{C})$ , a collection of *morphisms* (sometimes called arrows), that is, maps between the objects. We use

$$\text{hom}_{\mathcal{C}}(A, B) = \{f | f : A \rightarrow B, A, B \in \text{ob}(\mathcal{C})\} \subset \text{hom}(\mathcal{C}) \quad (4)$$

to denote the collection of all morphisms from  $A$  to  $B$  in the category.

3. *compositions* of morphisms, i.e., for every triple of objects  $A, B, C$ , the binary operation

$$\circ : \text{hom}_{\mathcal{C}}(B, C) \times \text{hom}_{\mathcal{C}}(A, B) \rightarrow \text{hom}_{\mathcal{C}}(A, C). \quad (5)$$

Furthermore, the components of  $\mathcal{C}$  must fulfill the following axioms:

- (i) Associativity of composition:  $(h \circ g) \circ f = h \circ (g \circ f)$  holds for all morphisms  $f \in \text{hom}_{\mathcal{C}}(A, B)$ ,  $g \in \text{hom}_{\mathcal{C}}(B, C)$ ,  $h \in \text{hom}_{\mathcal{C}}(C, D)$ .
- (ii) Existence of identity morphisms: For each object  $A \in \text{ob}(\mathcal{C})$  there is an identity morphism  $1_A \in \text{hom}_{\mathcal{C}}(A, A)$  such that for every morphism  $f \in \text{hom}_{\mathcal{C}}(A, B)$  we have  $1_B \circ f = f \circ 1_A = f$ . (It can readily be shown that the identity morphisms are unique.)

An *isomorphism* is an invertible morphism. The map  $f \in \text{hom}_{\mathcal{C}}(A, B)$  is an isomorphism iff  $\exists g \in \text{hom}_{\mathcal{C}}(B, A)$  for which  $g \circ f = 1_A$  and  $f \circ g = 1_B$ . This makes  $f$  and  $g$  each others' inverses.

We will build on this basic definition in several key stages. The first is the notion of strict monoidal category. A *strict monoidal* category is a category equipped with an associative *tensor product*  $\otimes$ , which preserves the relationship between the objects and the morphisms, and has a unit object  $\mathbf{1} \in \text{ob}(\mathcal{C})$ .

Adding a family of natural symmetry isomorphisms  $\sigma_{A,B}$  with  $\sigma_{B,A} \circ \sigma_{A,B} = 1_A \otimes 1_B$  makes a monoidal category *symmetric*. Intuitively the symmetry isomorphisms mean that the relative order of the objects in a tensor product carries no fundamental significance.

A *compact closed* category is a symmetric monoidal category in which for each object  $A \in \text{ob}(\mathcal{C})$  there is a *dual object*  $A^* \in \text{ob}(\mathcal{C})$ , and the *unit* and *counit* morphisms  $\eta_A : \mathbf{1} \rightarrow A^* \otimes A$  and  $\epsilon_A : A \otimes A^* \rightarrow \mathbf{1}$ . In a sense the unit and counit morphisms correspond to entangled states.

Finally, a *dagger* compact closed category is a compact closed category that comes equipped with the *dagger functor* [10], which captures the notion of adjoint. It is an involution that associates every morphism  $f : A \rightarrow B$  with its *adjoint* morphism  $f^\dagger : B \rightarrow A$ , and is compatible with both the composition and the tensor product. The dagger functor behaves precisely in the way one would expect from the Hermitian adjoint operation on a Hilbert space. To make the analogy even stronger, an isomorphism  $f : A \rightarrow B$  is said to be *unitary* iff  $f^\dagger = f^{-1}$ .

### III. EXTENDED QUANTUM CIRCUIT DIAGRAMS

We will now begin our presentation of an extended form of the existing diagrammatic notation for describing quantum circuits. Some of these concepts were first introduced in [10, 17, 20], where the authors derived a categorical representation that was expressive enough to represent many of the components used in standard quantum circuits. In a seemingly independent research track, some of these concepts [10, 17, 20] also appeared in [3, 4] as well as related work.

Each extended quantum circuit diagram corresponds to a morphism in the category QC. The main difference to ordinary QCDs is that *an extended diagram does not have to correspond to a quantum operation*. One of the most important properties of these diagrams is that they can be manipulated in a very intuitive, visual way. Objects (e.g. boxes etc.) on wires can be slid along them: note that going around a curve takes a transpose. The wires themselves can be bent and rearranged. Nodes where several wires meet can often be combined and split according to simple rules. After such changes, the diagram can be converted back into an ordinary, physically implementable quantum circuit, depending on the specific application.

**Definition 2** (The category of quantum circuits QC). QC is a category that consists of

1. Objects  $A = \{\mathcal{A}, D_A\}$ , where  $\mathcal{A}$  is a finite dimensional complex Hilbert space and  $D_A = (d_{A_i})_i$  a list of integer dimensions such that  $\dim \mathcal{A} = \prod_i d_{A_i}$ .
2. Morphisms  $f : A \rightarrow B$ , bounded linear maps between the finite dimensional Hilbert spaces  $\mathcal{A}$  and  $\mathcal{B}$ .  $D_A$  and  $D_B$  are the input and output dimensions of the morphism, respectively.<sup>2</sup>
3. Composition of morphisms  $\circ$ , which is just the usual composition of linear maps.
4. Tensor product bifunctor  $\otimes$  with the unit object  $\mathbf{1} = \{\mathbb{C}, (1)\}$ .  $A \otimes B := \{\mathcal{A} \otimes \mathcal{B}, D_A \star D_B\}$ , where  $\star$  denotes list concatenation with the elimination of singleton dimensions, and  $f \otimes g$  has its usual meaning.
5. Dagger functor  $\dagger$ , which is identity on the objects and takes the Hermitian adjoint of the morphisms.
6. Dual functor  $*$ , which is identity on the objects and takes the transpose of the morphisms in the computational basis. The unit and counit morphisms are likewise defined in terms of the computational basis:  $\eta_A = \sum_k |k, k\rangle$ ,  $\epsilon_A = \eta_A^\dagger$ .

**Theorem 3.** QC is a dagger compact closed category

*Proof.* It is straightforward to show that QC is a category: composition of the morphisms is clearly associative, and for each object  $A$  the corresponding identity morphism  $1_A$  is the identity map  $\mathbb{1}_A$  on  $\mathcal{A}$ .

QC is also readily seen to be strictly monoidal. The tensor product is associative, fulfills the bifunctor requirements, and  $\mathbf{1} \otimes A = A \otimes \mathbf{1} = A$ . The associator and left and right unitor isomorphisms are given by  $\alpha_{ABC} = \mathbb{1}_{A \otimes B \otimes C}$  and  $\lambda_A = \rho_A = \mathbb{1}_A$ .

The symmetric braiding isomorphism  $c_{A,B} : A \otimes B \rightarrow B \otimes A$ , required to make QC symmetric monoidal, is given by the SWAP gate:  $c_{A,B} = \sum_{ab} |ba\rangle_{B,A} \langle ab|_{A,B}$ .

The dagger is a contravariant endofunctor, is easily seen to be involutive and has the proper interaction with the composition and tensor product:  $1_A^\dagger = 1_A$ ,  $(g \circ f)^\dagger = f^\dagger \circ g^\dagger$ , and  $(f \otimes g)^\dagger = f^\dagger \otimes g^\dagger$ . Furthermore  $\alpha$ ,  $\lambda$ ,  $\rho$  and  $c$  are all unitary, so QC is dagger symmetric monoidal.

The dual is a contravariant endofunctor and the unit and counit morphisms fulfill the adjunction triangles (“snake equations”), and are symmetric. Together with the other properties this makes QC a dagger compact closed category.  $\square$

A unitary QC-morphism is also called a *gate*.

**Remark 4** (Quantum circuits as PROPs). We have placed the dagger compact closed structure into a list in Definition 2 (which is essentially a free construction). This is motivated for conceptual understanding as quantum computations typically take place in a fixed Hilbert space with each subsystem labeled. Symmetric monoidal categories with fixed types (e.g. all the objects are say qubits) are called PROPs [21]. We won’t use PROPs however, since this would limit say talking about objects or morphisms on qubits composed with qutrits.

**Remark 5** (Basic notational differences to standard string diagrams). To make our presentation more approachable to readers who have a background in quantum information science (as opposed to category theory), we have decided to depart from certain common category theory conventions.

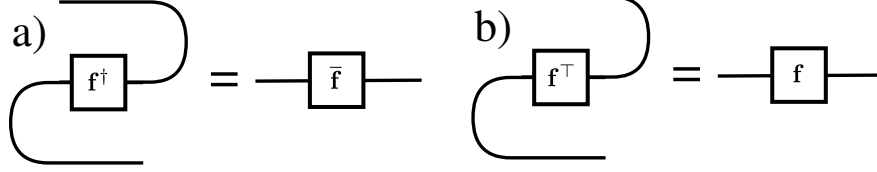
- As is the case of standard QCDs, in the present diagrams time flows from left to right across the page. This is in contrast to the diagrams in some category theory texts in which time flows either downwards or upwards.
- In addition to the usual unit and counit morphisms  $\eta$  and  $\epsilon$  we define the corresponding normalized states and costates:  $|\cup\rangle_{\mathcal{A}} = \frac{1}{\sqrt{d}} \eta_{\mathcal{A}}$  and  $\langle \cup|_{\mathcal{A}} = \frac{1}{\sqrt{d}} \epsilon_{\mathcal{A}}$ , where  $d = \dim \mathcal{A}$ . They correspond to physically realizable entangled states and help to keep the normalization of the diagrams explicit.
- Also, we do not use dual spaces in implementing the compact structures but rather choose a preferred *computational basis*, as is common in quantum computing. Hence our wires do not have directional markers on them.

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<sup>2</sup> We will often call QC-morphisms “tensors” depending on context.

**Remark 6** (Fixing a basis). Any vector space  $\mathcal{V}$  has a dual  $\mathcal{V}^*$ , the space of linear functions from  $\mathcal{V}$  to the ground field  $\mathbb{K}$ , that is  $f : \mathcal{V} \rightarrow \mathbb{K}$ . We must however fix a basis to identify the vector space  $\mathcal{V}$  with its dual. A basis  $\{|e_i\rangle\}_i$  in  $\mathcal{V}$  defines a dual basis  $\{\langle f_j|\}_j$  in  $\mathcal{V}^*$  through  $\langle f_j|e_i\rangle = \delta_{ij}$ . This defines an isomorphism  $\mathcal{V} \rightarrow \mathcal{V}^*$ ,  $|e_i\rangle \mapsto \langle f_i|$ , and allows us to identify  $\mathcal{V}^*$  with  $\mathcal{V}$ . In the present work, we will fix the canonical basis (called the computational basis in quantum information science).

**Definition 7** (Diagrammatic adjoints). As mentioned, cups and caps allow us to take the transpose of a linear map (b); and (a) following the (now) standard string diagram literature we introduce the derived concept of adjoint [10].



## A. Basic definitions

In this section we introduce key concepts that are used throughout the paper.

**Remark 8** (Einstein summation notation). We make use of Einstein notation for covariant and contravariant tensor indices, along with the usual summation convention (indices appearing once as a subscript and once as a superscript in the same term are summed over) whenever the summation limits are evident from the context.

**Definition 9** (Computational basis). For each  $d$ -dimensional Hilbert space  $\mathcal{H}$  we encounter we shall choose a computational basis, which we denote by  $\{|i\rangle_{\mathcal{H}}\}_{i=0}^{d-1}$ .

Modular arithmetic can be handled by introducing a congruence relation on the integers that is compatible with the operations of the ring of integers: addition, subtraction, and multiplication which behave an interact in the standard way. We use modulo  $d$  arithmetic for the basis vector indices, using the symbols  $\oplus$  and  $\ominus$  to denote modular addition and subtraction. When necessary, a subscript outside an operator, a ket or a bra is introduced to denote the subsystem to which it acts or corresponds.

**Definition 10** (Discrete Fourier transform gate). We denote the discrete Fourier transform gate by  $H$ :

$$H_{\mathcal{H}} := \frac{1}{\sqrt{d}} \sum_{ab} e^{i2\pi ab/d} |a\rangle\langle b|, \quad (6)$$

where  $d = \dim \mathcal{H}$  is the dimension of the Hilbert space the gate acts in. We can see that  $H^T = H$ , and that in a qubit system  $H$  coincides with the one-qubit Hadamard gate.

**Definition 11** ( $x$ -basis). Essentially the discrete fourier transform  $H$  is a transformation between two mutually unbiased bases, the computational basis and the  $x$ -basis  $\{|x_k\rangle\}_{k=0}^{d-1}$ , defined as

$$|x_k\rangle := H|k\rangle. \quad (7)$$

**Definition 12** (Negation gate). The negation gate is defined as

$$\ominus_{\mathcal{H}} := H_{\mathcal{H}}^2 = H_{\mathcal{H}}^{\dagger 2} = \sum_a |\ominus a\rangle\langle a|_{\mathcal{H}}. \quad (8)$$

As the name suggests, it performs a negation modulo  $d$  in the computational basis. As one would expect we have  $\ominus^2 = H^4 = \mathbb{1}$ , as shown in Fig. 1. In a qubit system the negation gate is equal to the identity operator.

**Definition 13** (Generalized  $Z$  and  $X$  gates). Given a Hilbert space  $\mathcal{H}$  and a computational basis, we define the generalized  $Z$  and  $X$  gates as follows:

$$Z_{\mathcal{H}} := \sum_k e^{i2\pi k/d} |k\rangle\langle k| \quad \text{where } d = \dim \mathcal{H}, \quad (9)$$

$$X_{\mathcal{H}} := \sum_k |k \oplus 1\rangle\langle k|. \quad (10)$$

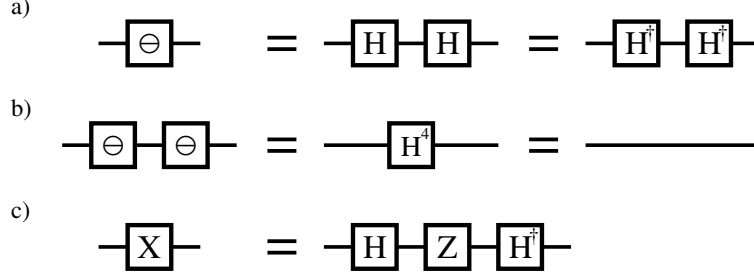


FIG. 1. Basic utility gates. (a) The  $\ominus$  gate performs a modular negation in the computational basis.  $\ominus : |k\rangle \mapsto |\ominus k\rangle$ . It can be implemented using the discrete Fourier transform gate  $H$ . (b) Negation gate squared equals identity:  $\ominus^2 = H^4 = \mathbb{1}$ . (c) The  $X$  gate modularly increments by one in the computational basis:  $X : |k\rangle \mapsto |k \oplus 1\rangle$ . The  $Z$  gate does the same in the  $x$ -basis.

In fact the  $Z$  and  $X$  gates are the same operator in two different bases, related through conjugation with  $H$ :

$$HXH^\dagger = Z, \quad (11)$$

$$HZH^\dagger = X^{-1}. \quad (12)$$

$X$  has the  $x$ -basis as its eigenbasis and modularly increments a computational basis state by 1, whereas  $Z$  is diagonal in the computational basis and modularly increments  $x$ -basis states:

$$X^a |k\rangle = |k \oplus a\rangle, \quad (13)$$

$$Z^a |x_k\rangle = HX^a H^\dagger H |k\rangle = H |k \oplus a\rangle = |x_{k \oplus a}\rangle. \quad (14)$$

Furthermore, we have

$$Z^a X^b = e^{i2\pi ab/d} X^b Z^a \quad \text{and} \quad (15)$$

$$\text{Tr}(Z^a X^b) = d \delta_{a,0} \delta_{b,0}. \quad (16)$$

Fig. 1 presents the gate symbols we use for the  $Z$  and  $X$  gates. When  $\mathcal{H}$  is a qubit,  $X$  and  $Z$  reduce to the Pauli matrices  $\sigma_x$  and  $\sigma_z$ , respectively.

**Definition 14** (Modular adder gate). We define the modular adder gate

$$\text{ADD}_{i,j} := \sum_{xy} |x, y \oplus x\rangle \langle x, y|_{i,j}. \quad (17)$$

The negated modular adder gate, NADD, is obtained by negating the “result qudit” of the ADD gate:

$$\text{NADD}_{i,j} := \ominus_j \text{ADD}_{i,j} = \sum_{xy} |x, \ominus x \ominus y\rangle \langle x, y|_{i,j}. \quad (18)$$

In a two qubit system both ADD and NADD reduce to the CNOT gate, and thus can be understood as its generalizations. NADD is self-inverse while ADD is not, which is why we choose to use the traditional CNOT symbol to denote NADD in general. For ADD we add a small arrow to denote the output direction. Fig. 2 presents the gate symbol and identities involving ADD, NADD and  $H$ .

**Definition 15** (Generalized plus state). We define the generalized  $|+\rangle_{\mathcal{H}}$  state as

$$|+\rangle_{\mathcal{H}} := |x_0\rangle_{\mathcal{H}} = H|0\rangle_{\mathcal{H}} = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |i\rangle_{\mathcal{H}}, \quad \text{where } d = \dim \mathcal{H}. \quad (19)$$

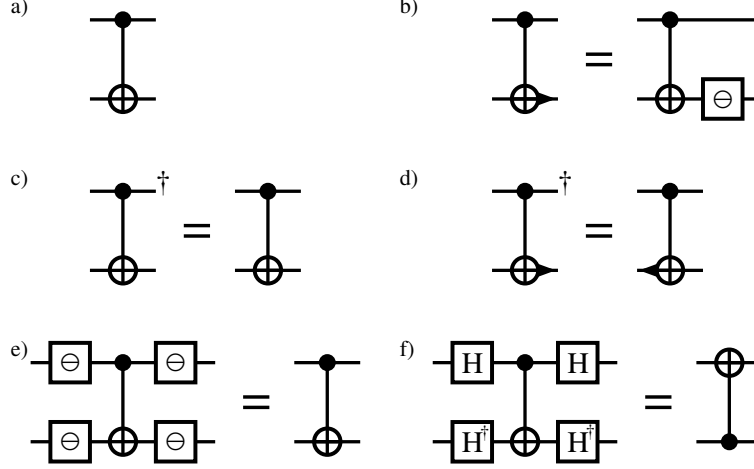


FIG. 2. (a) NADD gate:  $|x, y\rangle \mapsto |x, \ominus x \ominus y\rangle$ . (b) ADD gate:  $|x, y\rangle \mapsto |x, x \oplus y\rangle$ . (c,d) NADD is self-inverse, ADD is not, hence the need for the arrow-like symbol denoting the output direction. (e,f) Identities involving NADD,  $\ominus$  and  $H$ .

**Definition 16** (Generalised Bell states). The concept of Bell state, normally defined for two-qubit systems, can be generalized to systems of two  $d$ -dimensional qudits. In this case the Bell states  $\{|B_{a,b}\rangle\}_{a,b=0}^{d-1}$  are a set of  $d^2$  orthonormal and maximally entangled two-qudit states. They are parametrized by two integers,  $a$  and  $b$ , and can be prepared using the circuit in Fig. 3:

$$|B_{a,b}\rangle_{\mathcal{H}\otimes\mathcal{H}} := \frac{1}{\sqrt{d}} \sum_k e^{i2\pi ak/d} |k, k \oplus b\rangle = \text{ADD}_{1,2} H_1 |a, b\rangle_{1,2}. \quad (20)$$

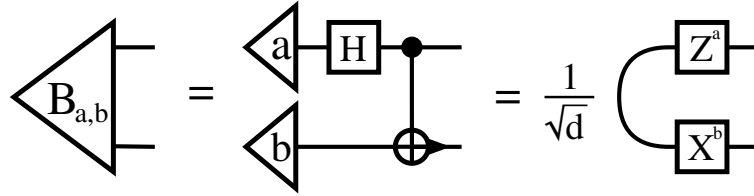


FIG. 3. Generalized Bell states. Preparation using the ADD gate, relation to the cup element (see Sec. III D).

We will now proceed to describe the basic elements appearing in the extended QCDs.

### B. Systems as QC-objects

In our diagrams, much like in ordinary QCDs, time flows from left to right.<sup>3</sup> Horizontal wires each describe individual quantum systems (complex Hilbert spaces). Stacking these wires vertically corresponds to a composite system (a QC-object comprised of several Hilbert spaces). Alternatively, a wire  $\mathcal{A}$  can be understood as the identity morphism  $1_{\mathcal{A}}$ . The unit object for the tensor product,  $\mathbf{1}$ , is represented by empty space.

<sup>3</sup> In converting a diagram into an algebraic expression one naturally needs to reverse the left-right order since traditional quantum mechanics uses left multiplication to represent operations on states.



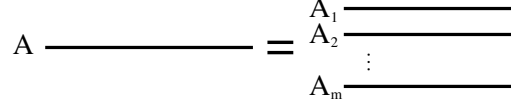


FIG. 4. Two equivalent descriptions of the system with the Hilbert space  $\mathcal{A} = \mathcal{A}_1 \otimes \mathcal{A}_2 \otimes \dots \otimes \mathcal{A}_m$ .

Unless it is clear from the context, the dimension of each wire should be explicitly stated, especially if they're not all equivalent. Also, since a larger Hilbert space often can be factored into a tensor product of subsystems in many different ways, there may be more than one equivalent description of a composite system in terms of wires, as illustrated in Fig. 4. Each such description corresponds to an object in the category QC.

Unlike in standard QCDs, the wires are allowed to deviate from a straight horizontal line and even cross each other (which corresponds to swapping the order of the corresponding subsystems), as long as they remain *progressive* from left to right. As we shall later see, a wire reversing its direction of progression has a special meaning.

### C. Morphisms: states and operators on equivalent footing

Category theory allows one to study the mathematical structure formed not only by the composition of processes but also the composition of states. This becomes evident once we define both states and operators as morphisms in the category. In the diagrams the morphisms are represented by geometrical shapes connected to the wires.<sup>4</sup>

#### 1. States as QC-morphisms

In QC, a pure state  $|\psi\rangle \in \mathcal{A}$  (represented by a ket, or a ray in the Hilbert space) corresponds to a linear map  $\psi$  from the unit of the tensor product  $\mathbf{1}(=\mathbb{C})$  to  $\mathcal{A}$ , or the morphism

$$\psi : \mathbf{1} \rightarrow \mathcal{A}, \quad z \mapsto z|\psi\rangle. \quad (21)$$

For instance, consider the two-qubit state  $|\Psi_+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$ : this corresponds to the morphism  $\mathbb{C} \xrightarrow{\Psi_+} \mathcal{H}_2 \otimes \mathcal{H}_2$  in the category.

In a diagram a pure state (or equivalently the corresponding state preparation procedure) is represented by a left-pointing labeled triangle with a number of wires extending from its base to the right, as shown in Fig. 5. Each wire corresponds to a subsystem of the state. Flipping a triangle horizontally converts it into the corresponding costate (bra), and can be understood as a projective measurement with postselection (an *effect*).

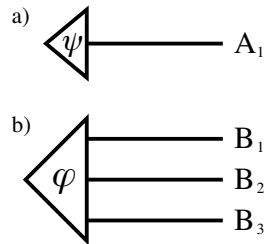


FIG. 5. (a) State  $|\psi\rangle$  with a single subsystem. (b) State  $|\varphi\rangle$  with three subsystems.  $|\psi\rangle$  is a map of type  $\mathbf{1} \rightarrow \mathcal{A}_1$  and  $|\varphi\rangle$  is a map of type  $\mathbf{1} \rightarrow \mathcal{B}_1 \otimes \mathcal{B}_2 \otimes \mathcal{B}_3$ .

<sup>4</sup> The one exception to this rule are morphisms of the type  $f : \mathbf{1} \rightarrow \mathbf{1}$ , also called *scalars*. Since the tensor unit object  $\mathbf{1}$  is represented by empty space, the representation for  $f$  is a geometric shape not connected to anything.

A state  $|\psi\rangle$  can be expanded in the computational bases of its component systems, resulting in the presentation

$$|\psi\rangle = \psi^{a_1 \dots a_m} |a_1 \dots a_m\rangle \in \mathcal{A}_1 \otimes \mathcal{A}_2 \otimes \dots \otimes \mathcal{A}_m. \quad (22)$$

## 2. Operators as QC-morphisms

Operators, or bounded linear maps from one Hilbert space to another, can be naturally identified with the morphisms in QC. As an example we can consider quantum gates, unitary maps from a Hilbert space to itself.

In the diagrams operators are represented using labeled boxes on the wires, as shown in Fig. 6. Assume that we have a map  $f : \mathcal{A} \rightarrow \mathcal{B}$ . The domain and codomain are tensor products of finite dimensional Hilbert spaces given by  $\mathcal{A} = \mathcal{A}_1 \otimes \mathcal{A}_2 \otimes \dots \otimes \mathcal{A}_m$  and  $\mathcal{B} = \mathcal{B}_1 \otimes \mathcal{B}_2 \otimes \dots \otimes \mathcal{B}_n$ . This means that the diagram for  $f$  has  $m$  input legs and  $n$  output legs. For certain operators, such as the ADD gate, we use specific symbols.

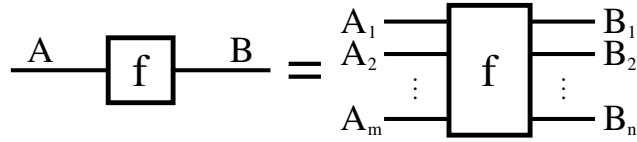


FIG. 6. Map  $f : \mathcal{A} \rightarrow \mathcal{B}$ .

Using the computational bases defined on the component spaces, we can present  $f$  as

$$f = |b_1 \dots b_n\rangle \langle b_1 \dots b_n| f |a_1 \dots a_m\rangle \langle a_1 \dots a_m| = |b_1 \dots b_n\rangle f^{b_1 \dots b_n}_{a_1 \dots a_m} \langle a_1 \dots a_m|. \quad (23)$$

Given a state  $|\psi\rangle = \psi^{a_1 \dots a_m} |a_1 \dots a_m\rangle \in \mathcal{A}$ , we have  $f|\psi\rangle = f^{b_1 \dots b_n}_{a_1 \dots a_m} \psi^{a_1 \dots a_m} |b_1 \dots b_n\rangle \in \mathcal{B}$ .

## 3. Composition and tensor product

The category QC has two composition-like operations, the the tensor product  $\otimes$ , and the composition of morphisms  $\circ$ . The composition of morphisms is represented graphically by the sequential composition of the corresponding diagram elements and connecting the corresponding wires. Likewise, tensor products of objects or morphisms is represented by the vertical stacking of the diagram elements. These diagrammatic structures are illustrated in Fig. 7.

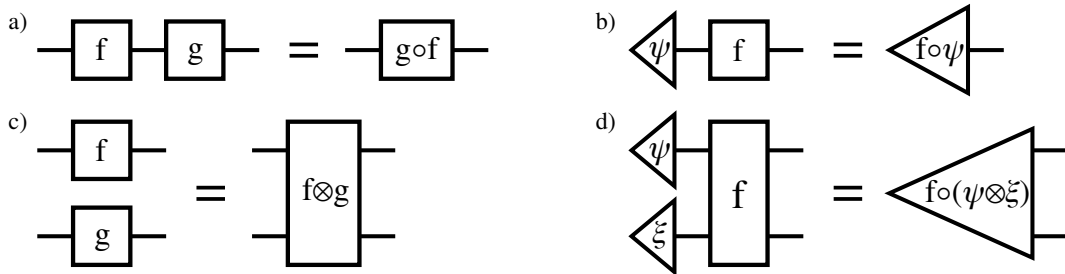


FIG. 7. Composition and tensor product. (a) Composition of operators.  $(g \circ f)^a_c = g^a_b f^b_c$ . (b) Composition of a state and an operator.  $(f \circ \psi)^a = f^a_b \psi^b$ . (c) Tensor product of operators.  $(f \otimes g)^{ac}_{bd} = f^a_b g^c_d$ . (d) Tensor product of states composited with an operator.  $(f \circ (\psi \otimes \xi))^{a_1 a_2} = f^{a_1 a_2}_{b_1 b_2} \psi^{b_1} \xi^{b_2}$ .

**Remark 17** (Bifactoriality [22]). In the diagrammatic calculus, the equation

$$(g \circ f) \otimes (t \circ s) = (g \otimes t) \circ (f \otimes s) \quad (24)$$

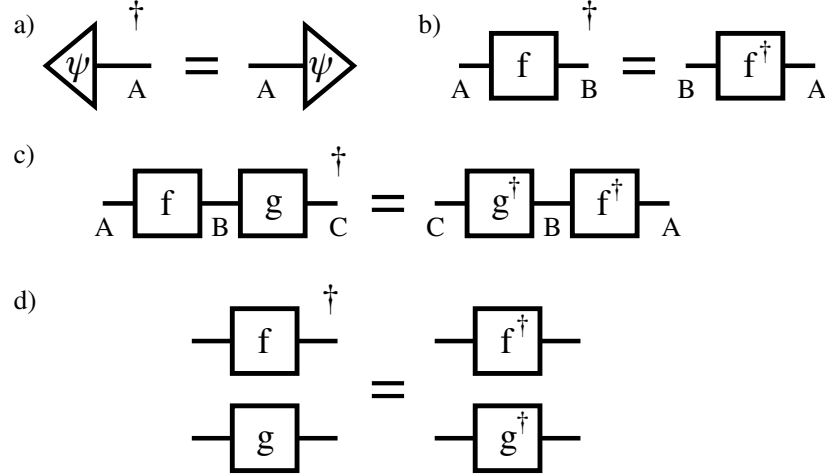


FIG. 8. Dagger functor. (a) Dagger of a state.  $(\psi^\dagger)_a = \psi_a^*$ . (b) Dagger of an operator.  $(f^\dagger)^a_b = f_b^{a*}$ . (c) Dagger of composition.  $(g \circ f)^\dagger = f^\dagger \circ g^\dagger$ . (d) Dagger of tensor product.  $(f \otimes g)^\dagger = f^\dagger \otimes g^\dagger$ .

has the evident pictorial meaning which amounts to first connecting boxes horizontally (resulting in  $g \circ f$ ,  $t \circ s$ ), and then stacking them vertically to yield  $(g \circ f) \otimes (t \circ s)$ , or first stacking them vertically (resulting in  $g \otimes t$ ,  $f \otimes s$ ), and then connecting the stacks horizontally to yield  $(g \otimes t) \circ (f \otimes s)$ .

#### 4. The dagger functor

The effect of the dagger functor in the category QC, taking the Hermitian conjugate of a morphism, is represented diagrammatically by mirroring the diagram in the horizontal direction. Hence given a morphism  $f$ , the diagrams corresponding to  $f$  and  $f^\dagger$  are each others' mirror images. The operator labels get a  $\dagger$  symbol appended whereas the state and costate symbols stay the same. This is illustrated in Fig. 8.

#### D. Cups and caps: Bell states and Bell effects

We will now make use of the structure of compact closure (see the definition of dagger-compact closure [10] as well as the more accessible read [19]) to derive elegant dualities between morphisms of different types. This provides an intuitive generalization of concepts surrounding the Choi-Jamiołkowski isomorphism.

Following ideas in [10], we introduce two new diagrammatic structures that do not appear in standard quantum circuits, shown in Fig. 9. They are the only ways a wire may reverse its direction of left-right

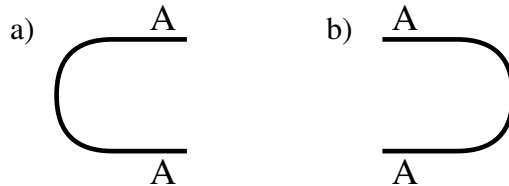


FIG. 9. Dagger-compact structures. (a) Cup  $\eta_A$ . (b) Cap  $\epsilon_A$ .

progression.

The first one, called a *cup*, is simply another way of denoting a state preparation procedure for a generalized Bell state in the Hilbert space  $\mathcal{A}^{\otimes 2}$ , scaled by  $\sqrt{d_A}$  where  $d_A = \dim \mathcal{A}$ .

**Definition 18** (Cup). The cup is the diagram element that corresponds to the dagger-compact structure  $\eta$

of the category **QC**. It is a morphism  $\eta_{\mathcal{A}} : \mathbf{1} \rightarrow \mathcal{A} \otimes \mathcal{A}$ , given in the computational basis as

$$\eta_{\mathcal{A}} := \sum_{i=0}^{d_{\mathcal{A}}-1} |i\rangle_{\mathcal{A}} \otimes |i\rangle_{\mathcal{A}} = \delta^{ij} |ij\rangle_{\mathcal{A} \otimes \mathcal{A}}. \quad (25)$$

It is easy to notice that  $\eta_{\mathcal{A}}$  is proportional to the  $(0,0)$  Bell state we defined previously:

$$|\cup\rangle_{\mathcal{A}} := \frac{1}{\sqrt{d_{\mathcal{A}}}} \eta_{\mathcal{A}} = |B_{0,0}\rangle_{\mathcal{A} \otimes \mathcal{A}}, \quad (26)$$

and that the other Bell states are locally equivalent to  $|\cup\rangle$ , as shown in Fig. 3.

The *cap* can be thought of physically as corresponding to a postselected measurement (an effect) in the generalized Bell basis.

**Definition 19** (Cap). The cap is the diagram element that corresponds to the dagger-compact structure  $\epsilon$  of the category **QC**. It is obtained by taking the dagger of the cup, which makes it the morphism  $\epsilon_{\mathcal{A}} : \mathcal{A} \otimes \mathcal{A} \rightarrow \mathbf{1}$ :

$$\epsilon_{\mathcal{A}} := \eta_{\mathcal{A}}^{\dagger} = \sum_{i=0}^{d_{\mathcal{A}}-1} \langle i|_{\mathcal{A}} \otimes \langle i|_{\mathcal{A}} = \delta_{ij} \langle ij|_{\mathcal{A} \otimes \mathcal{A}}. \quad (27)$$

One may safely think that the purpose of these structures is to entangle two subsystems in a way that enables very intuitive manipulation of the corresponding circuit diagrams by bending the wires in them. This is based on isomorphisms they induce between states and operators.

Now we'll demonstrate some properties of these circuit elements, corresponding to the diagram identities in Fig. 10. We give proofs for cups, but corresponding identities hold for caps as well, and the proofs can be obtained by taking the Hermitian conjugates of the ones we give below.

**Theorem 20** (Cup and cap symmetry (Fig. 10a)). *Since the cup corresponds to a symmetric state, it immediately follows that the relative order of the two subsystems is irrelevant. Diagrammatically this means the order of the wires can be swapped.*

**Theorem 21** (Sliding operators around cups and caps (Fig. 10b)). *An operator  $f : \mathcal{A} \rightarrow \mathcal{B}$  can be moved ("slid") around a cup or a cap by transposing it in the computational basis. Alternatively, there is an isomorphism between a cup followed by the operator  $f$  on the first subsystem, the state  $|\tilde{f}\rangle := \frac{1}{\sqrt{d_{\mathcal{A}}}} \text{vec}(f^T)^k |k\rangle_{\mathcal{B} \otimes \mathcal{A}}$ , and a cup followed by the operator  $f^T$  on the second subsystem.*<sup>5</sup>

*Proof.*

$$\begin{aligned} (f_j^i |i\rangle \langle j|_1) \eta_{\mathcal{A}1,2} &= (f_j^i |i\rangle \langle j|_1) (\delta^{kl} |k\rangle_1 |l\rangle_2) = f_j^i \delta_j^k \delta^{kl} |i\rangle_1 |l\rangle_2 \\ &= f_j^{ij} |i\rangle_1 |j\rangle_2 = \text{vec}(f^T)^k |k\rangle_{1,2} = \sqrt{d_{\mathcal{A}}} |\tilde{f}\rangle_{1,2} = f_j^i \delta_l^j \delta^{kl} |k\rangle_1 |i\rangle_2 \\ &= (f_j^i |i\rangle \langle j|_2) (\delta^{kl} |k\rangle_1 |l\rangle_2) = ((f^T)^i_j |i\rangle \langle j|_2) \eta_{\mathcal{B}1,2} \end{aligned} \quad (28)$$

□

**Corollary 22.** *All local unitary operators  $f$  are isomorphic to a state  $|\tilde{f}\rangle$  that is locally equivalent to a generalized Bell state.*

**Corollary 23** (Conversions between inputs and outputs of the same type). *More generally, a cup converts an input leg of an operator into an output leg of same type. The opposite is true for a cap.*

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<sup>5</sup> The *vec* operation takes the matrix of its operand in the computational basis and rearranges it column by column, left to right, into a column vector.

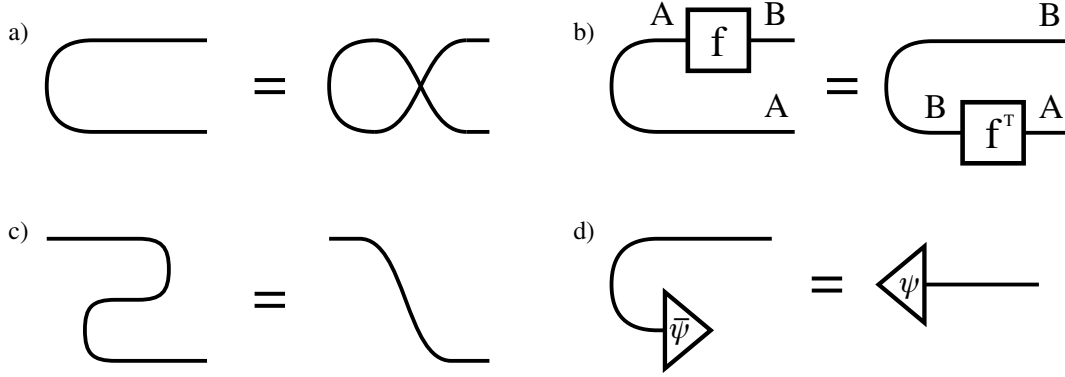


FIG. 10. Cup identities. (a) Symmetry. (b) “Sliding” an operator around a cup transposes it in the computational basis. (c) Teleportation or the “snake equation”. (d) Conjugate state.

*Proof.*

$$\begin{aligned}
 (f \otimes \mathbb{1}_\omega) \eta_{q,\omega} &= (|b_1 \cdots b_n\rangle \otimes |x\rangle_\omega f^{b_1 \cdots b_n}_{a_1 \cdots a_m} \langle a_1 \cdots a_m| \otimes \langle x|_\omega) (\delta^{kl} |k\rangle_q |l\rangle_\omega) \\
 &= |b_1 \cdots b_n\rangle \otimes |x\rangle_\omega f^{b_1 \cdots b_n}_{a_1 \cdots a_m} \langle a_1 \cdots a_{q-1} a_{q+1} \cdots a_m | \delta^{kl} \delta^{a_q}_k \delta^{x_l} \\
 &= |b_1 \cdots b_n\rangle \otimes |a_q\rangle_\omega f^{b_1 \cdots b_n}_{a_1 \cdots a_{q-1} a_{q+1} \cdots a_m} \langle a_1 \cdots a_{q-1} a_{q+1} \cdots a_m | \\
 &= |b_1 \cdots b_n\rangle \otimes |a_q\rangle_\omega f^{b_1 \cdots b_n a_q}_{a_1 \cdots a_{q-1} a_{q+1} \cdots a_m} \langle a_1 \cdots a_{q-1} a_{q+1} \cdots a_m |.
 \end{aligned} \tag{29}$$

□

**Theorem 24** (Snake equation (Fig. 10c)). *A cup and a cap can combine to cancel each other. In other words a double bend in a wire can be pulled straight. In Section IV B we show how this operation actually corresponds to the standard quantum teleportation protocol [10].*

*Proof.*

$$\begin{aligned}
 (\epsilon_{1,2} \otimes \mathbb{1}_3) (\mathbb{1}_1 \otimes \eta_{2,3}) &= (\delta_{ij} \langle i|_1 \langle j|_2 \otimes \mathbb{1}_3) (\mathbb{1}_1 \otimes \delta^{kl} |k\rangle_2 |l\rangle_3) \\
 &= \delta_{ij} \delta^{kl} \delta^j_k |l\rangle_3 \langle i|_1 = |i\rangle_3 \langle i|_1 = \mathbb{1}_{3,1}.
 \end{aligned} \tag{30}$$

□

**Theorem 25** (Conjugate states (Fig. 10d)). *Cups and caps introduce an isomorphism between states  $|\psi\rangle = \psi^k |k\rangle$  and their conjugate states  $\langle \bar{\psi}| := \langle k| \psi_k$ , which are obtained by complex conjugating the coefficients of the corresponding bra in the computational basis.*

*Proof.*

$$\langle \bar{\psi}|_2 \eta_{1,2} = (\psi_j \langle j|_2) (\delta^{kl} |k\rangle_1 |l\rangle_2) = \psi_j \delta^j_l \delta^{kl} |k\rangle_1 = \psi^k |k\rangle_1 = |\psi\rangle_1. \tag{31}$$

□

**Remark 26** (Basis dependence of transposition and complex conjugation). At first it might seem strange that we should encounter basis-dependent operations such as transposition and complex conjugation. However, this is a direct result of us having chosen a preferred computational basis and defining the cup/cap operators in terms of it.

## E. Dots

*Dots* are a subclass of operators. Most importantly, the definition for each type of dot is trivially extensible to an arbitrary number of input and output legs, all of which have the same dimension. A dot with  $n$  input legs and  $m$  output legs is called an  $n$ -to- $m$  dot and denoted  $\text{DOT}^{m \rightarrow n}$ . Furthermore, the dagger operation simply converts a dot’s input legs into output legs and vice versa:  $\text{DOT}^{m \rightarrow n\dagger} = \text{DOT}^{n \rightarrow m}$ .

### 1. Copy dots

**Definition 27** (COPY). Given an orthonormal basis  $B = \{|b_k\rangle\}_k$ , we define the 1-to-2 copy dot in this basis as

$$\text{COPY}_B^{1 \rightarrow 2} := \sum_k |b_k b_k\rangle \langle b_k|, \quad (32)$$

where we for clarity write the sum symbol explicitly since the index  $k$  appears three times in a term.

It is easy to see that given a state  $|b_k\rangle$  as the input,  $\text{COPY}_B^{1 \rightarrow 2}$  produces two copies of the same state as output.<sup>6</sup> Fig. 11 depicts several properties of COPY in diagram form.

For reasons that will become apparent, in our diagrammatic notation  $\text{COPY}^{1 \rightarrow 2}$  is represented by a circular node (“dot”) with one input leg, two output legs and a label identifying the basis in which it operates. The label is also called the *color* of the copy dot.

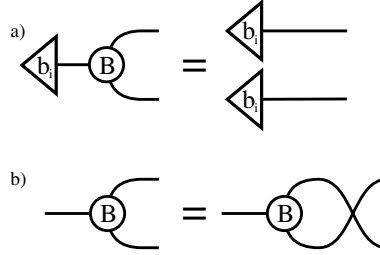


FIG. 11. Copy dot in the orthonormal basis  $B = \{|b_k\rangle\}_k$ . (a) Definition. (b) Symmetry.

**Remark 28** (COPY as a quantum operation).  $\text{COPY}_B^{1 \rightarrow 2}$  is a valid quantum operation since

$$\text{COPY}_B^{1 \rightarrow 2 \dagger} \text{COPY}_B^{1 \rightarrow 2} = \sum_{ij} |b_i\rangle \langle b_i b_i| b_j b_j \rangle \langle b_j| = \sum_i |b_i\rangle \langle b_i| = \mathbb{1}. \quad (33)$$

This however does not hold under the dagger —  $\text{COPY}_B^{1 \rightarrow 2 \dagger} = \text{COPY}_B^{2 \rightarrow 1}$  (*merge*) is not a valid quantum operation. It is however still useful to consider its properties — by invoking arguments such as postselection it can be given a physical meaning.

**Remark 29** (Copy dots with any number of legs). Copy dots are readily generalized to any number of input and output legs, all of which have the same dimension. An  $m$ -to- $n$  copy/merge dot in the basis  $B$  is given by

$$\text{COPY}_B^{m \rightarrow n} := \sum_k |\underbrace{b_k \cdots b_k}_n \rangle \langle \underbrace{b_k \cdots b_k}_m|. \quad (34)$$

It is a valid quantum operation iff  $m = 1$ .

**Definition 30** ( $\text{COPY}_Z$ ). As a special case, let us consider the copy dot in the computational basis. To conform with the standard quantum circuit notation, we denote it with a simple black dot  $\bullet$ :

$$\text{COPY}_Z^{1 \rightarrow 2} := \sum_k |kk\rangle \langle k| \quad (35)$$

**Remark 31** (Copy dots of arbitrary color). The unitary transformation from the computational basis to the basis  $B$ ,

$$U_B := \sum_k |b_k\rangle \langle k|, \quad (36)$$

can be used to convert a general  $\text{COPY}_B$  into a  $\text{COPY}_Z$ , as shown in Fig. 12.

<sup>6</sup> This does not violate the no cloning theorem since the operator can only faithfully copy a single fixed basis.

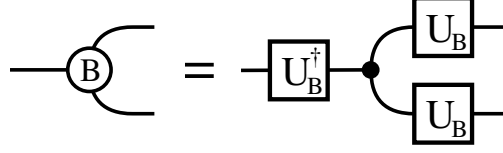


FIG. 12. Transformation between copy dots in different bases.  $U_B = \sum_k |b_k\rangle\langle k|$ .

### 2. Plus dots

**Definition 32** (PLUS). We define the plus dot with  $m$  input legs and  $n$  output legs, operating in the basis  $B$ , as

$$\text{PLUS}_B^{m \rightarrow n} := \text{COPY}_{H_B B}^{m \rightarrow n} \ominus_B^{\otimes m} = \frac{1}{d^{(m+n-2)/2}} \sum_{\substack{x_1 \dots x_m \\ y_1 \dots y_n}} \delta_{(\sum_i x_i \oplus \sum_j y_j), 0} |b_{y_1} \dots b_{y_n}\rangle \langle b_{x_1} \dots b_{x_m}|, \quad (37)$$

where  $H_B := U_B H U_B^\dagger$ ,  $\ominus_B := U_B \ominus U_B^\dagger$ , and  $d$  is the dimension of the legs. Specifically, for the plus dot in the computational basis we obtain the expression

$$\text{PLUS}_Z^{m \rightarrow n} = \text{COPY}_X^{m \rightarrow n} \ominus^{\otimes m} = \frac{1}{d^{(m+n-2)/2}} \sum_{\substack{x_1 \dots x_m \\ y_1 \dots y_n}} \delta_{(\sum_i x_i \oplus \sum_j y_j), 0} |y_1 \dots y_n\rangle \langle x_1 \dots x_m|. \quad (38)$$

Roughly speaking the plus dot makes sure all its inputs and outputs in the given basis sum to zero mod  $d$ . The plus dot is generally not a copy dot. Diagrammatically  $\text{PLUS}_Z$  is represented by the symbol  $\oplus$ .<sup>7</sup>

### 3. Spider law

Neighboring copy dots of the same color  $B$  can be merged into a single dot. In categorical quantum mechanics, this is called the spider law.

**Theorem 33** (Spider law [17]). *Given a connected graph with  $m$  inputs and  $n$  outputs comprised solely of Frobenius dots of equal dimension, this map can be equivalently expressed as a single  $m$ -to- $n$  dot, as shown in Fig. 13.*

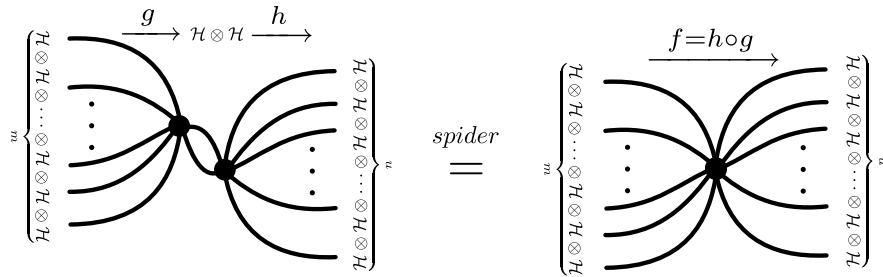


FIG. 13. Spider law.

The plus dots obey a slightly modified version of the spider law, in which all the connecting legs between two dots to be merged must have the negation gate  $\ominus_B$  on them.

<sup>7</sup> The diagrammatic representation of  $\text{PLUS}_Z^{1 \rightarrow 1}$  (a wire with  $\oplus$  on it) must not be confused with the notation occasionally used in standard QCDs, in which  $\oplus$  denotes the NOT gate. In our notation we instead have  $\text{PLUS}_Z^{1 \rightarrow 1} = \ominus$ . Note that we could have used this as the *definition* of the  $\ominus$  gate but felt this notational parsimony would not have been worth the potential confusion.

#### 4. Simplification rules

**Definition 34** (Unit element). A *unit element* for a dot is a state/costate which, when connected to a leg of the dot, gives a dot of the same type without that leg:

$$\text{DOT}_a^{m \rightarrow n} |\text{unit}_a\rangle = \text{DOT}_a^{(m-1) \rightarrow n}, \quad (39)$$

$$\langle \text{unit}_a | \text{DOT}_a^{m \rightarrow n} = \text{DOT}_a^{m \rightarrow (n-1)}. \quad (40)$$

It is easy to see that  $\sqrt{d}|0\rangle$  is a unit element for  $\text{PLUS}_Z$  (as well as for the  $\text{COPY}_X$ ) since it simply makes the corresponding index vanish in the Kronecker delta in Eq. (38). Using this result it is straightforward to show that  $\sqrt{d}|+\rangle$  is a unit element for  $\text{COPY}_Z$ . The interaction of the unit elements with their dots is presented in Fig. 14.

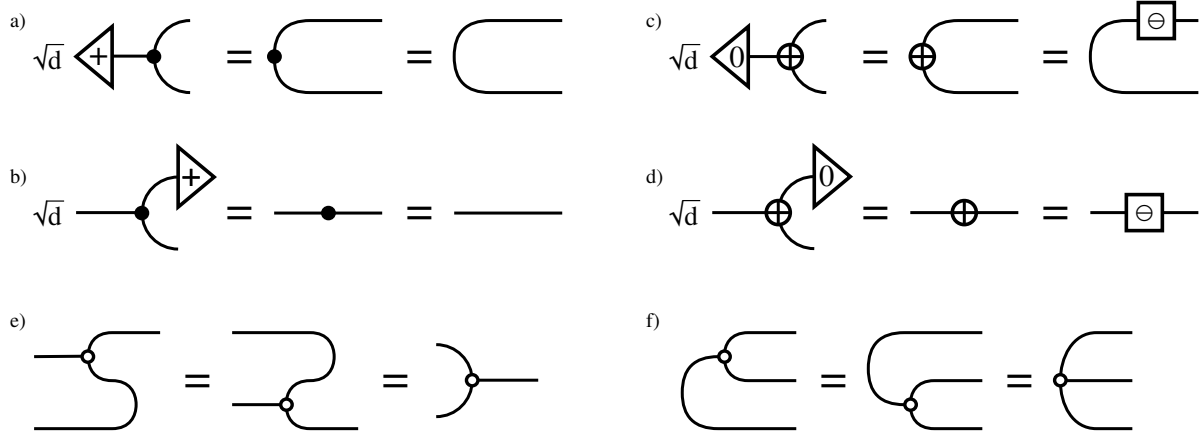


FIG. 14. Unit elements for the (a,b)  $\bullet$  and (c,d)  $\oplus$  dots. (e,f) Bending the legs of copy and plus dots using cups and caps. Here the empty dot refers to any copy or plus dot for which  $U_B = U_B^*$ , e.g. the  $\bullet$  and  $\oplus$  dots.

**Remark 35** (Induced dagger-compact structures). Three legged dots induce compact structures whenever there is a state or costate that, when connected to a leg of the dot, transforms it to a state locally equivalent to a cup or a cap.

**Remark 36** (Bending the legs of dots). By attaching one of the legs of a cup to an input leg of  $\text{COPY}_Z$  or  $\text{PLUS}_Z$  dot, we can see that the effect is to change it into an output leg. The same is of course true under the dagger.

$$\text{COPY}_Z^{m \rightarrow n} \eta = \text{COPY}_Z^{(m-1) \rightarrow (n+1)}, \quad (41)$$

$$\epsilon \text{COPY}_Z^{m \rightarrow n} = \text{COPY}_Z^{(m+1) \rightarrow (n-1)}. \quad (42)$$

This is illustrated in Fig. 14(e,f). This rule applies to general  $\text{COPY}_B$  and  $\text{PLUS}_B$  dots iff  $U_B = U_B^*$ .

**Theorem 37** (Commutation rules for the  $Z$  and  $X$  gates with dots). *Since the  $Z$  gate shares an eigenbasis with  $\text{COPY}_Z$ , they fully commute:*

$$\sum_k |k\rangle_1 |k\rangle_2 \langle k|_1 Z = \sum_k (Z|k\rangle_1) |k\rangle_2 \langle k|_1 = \sum_k |k\rangle_1 (Z|k\rangle_2) \langle k|_1. \quad (43)$$

The  $X$  gate, however, is duplicated when it passes a  $\text{COPY}_Z$ :

$$\sum_k |k\rangle_1 |k\rangle_2 \langle k|_1 X = \sum_k |k\rangle_1 |k\rangle_2 \langle k \oplus 1|_1 = \sum_k |k \oplus 1\rangle_1 |k \oplus 1\rangle_2 \langle k|_1 = \sum_k (X|k\rangle_1) (X|k\rangle_2) \langle k|_1 \quad (44)$$



One obtains equivalent results for  $\text{PLUS}_Z$  with the roles of  $Z$  and  $X$  exchanged. These commutation rules are presented in Fig. 15. Even though we used  $1 \rightarrow 2$  dots in our proofs above, analogous rules apply to  $\text{COPY}_Z$  and  $\text{PLUS}_Z$  dots with an arbitrary number of legs.<sup>8</sup>

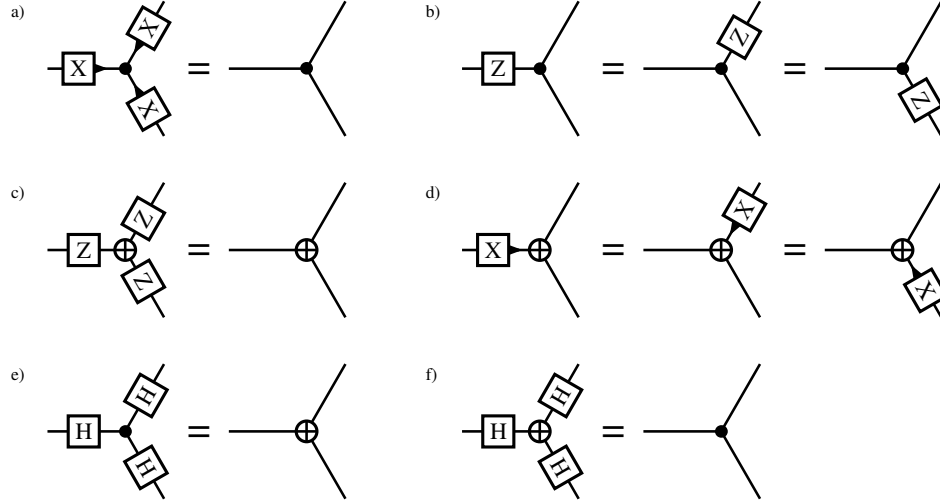


FIG. 15. Commutation rules for (a,b) the  $\bullet$  dot and (c,d) the  $\oplus$  dot with the  $Z$  and  $X$  gates. (e,f) Conversions between  $\bullet$  and  $\oplus$  dots using discrete Fourier transform gates  $H$ . Analogous rules apply to  $\bullet$  and  $\oplus$  dots with an arbitrary number of legs.

Now we have assembled all the necessary ingredients to make the dots do something useful. As the astute reader probably already has noticed, the notation we use for the  $\bullet$  and  $\oplus$  dots is suggestively similar to the NADD gate symbol, for a good reason. Fig. 16 shows how the NADD gate can be built out of dots, and how the  $\bullet$  and  $\oplus$  dots can be in some cases explicitly constructed using the NADD gate.

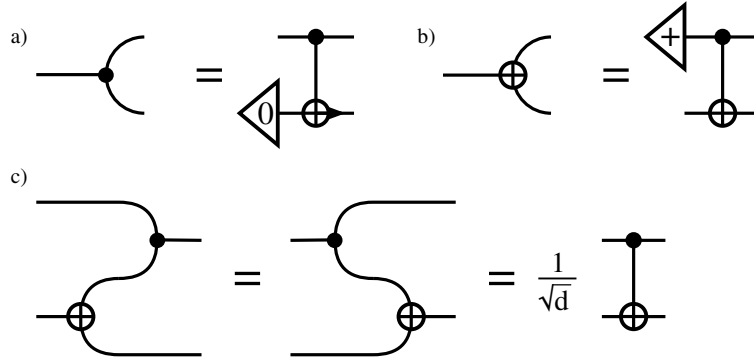


FIG. 16. (a–b) Explicit constructions for the  $\bullet$  and  $\oplus$  dots. (c) Combining the  $\bullet$  and  $\oplus$  dots yields NADD.

<sup>8</sup> Aesthetic interlude: Given the computational basis, the set of operations  $\{1, ^T, *, ^\dagger\}$  is isomorphic to the Klein group  $Z_2 \times Z_2$ , which also is the symmetry group of the rectangle. We can use this to illustrate the symmetry properties of operators with the symbols, by equating  $^T$  with a 180-degree rotation of the symbol,  $*$  with vertical reflection, and  $^\dagger$  with horizontal reflection. (This is analogous to the function of the corner marker on the morphism symbols in [12].) By adding an arrow to the  $X$  gate symbol to denote the direction of incrementation, together with the symmetries of the letter symbols themselves, we can see that the symmetry properties of the  $Z$  and  $X$  gates are exactly represented by the symmetries of their gate symbols:  $Z^T = Z$ ,  $X^* = X$ . The arrow would not be necessary if the symbol for the  $X$  gate had the correct symmetry in itself (like the letter  $E$ , for example), but we chose to go with the more traditional symbol.

### F. From diagrams to quantum operations

The extended QCDs each correspond to a QC-morphism. However, not every such morphism is physically implementable on its own. In quantum mechanics a state operator can (in principle) undergo any evolution that can be expressed as a linear, completely positive map (CPM). The mapping from QC-morphisms to CPMs is easiest achieved using the operator-sum representation, in which each morphism corresponds to a Kraus operator.

**Definition 38** (Complete set of QC-morphisms). We call a set of QC-morphisms  $S = \{f_i\}_i \subset \text{hom}_{\text{QC}}(A, B)$  *complete* iff it corresponds to a quantum operation, that is,

$$S \text{ is complete} \quad \Leftrightarrow \quad \sum_i f_i^\dagger f_i = 1_A. \quad (45)$$

The effect of  $S$  on the state operator  $\rho : \mathcal{A} \rightarrow \mathcal{A}$  is

$$\rho \mapsto \sum_i f_i \rho f_i^\dagger. \quad (46)$$

Another category-based approach to representing CPMs using diagrams can be found in [23].

**Lemma 39** (Properties of complete sets of QC-morphisms). *The following properties immediately follow from the definition:*

- (a) If  $f \in \text{hom}_{\text{QC}}(A, A)$  is unitary, it is complete on its own.
- (b) A state  $\psi : \mathbf{1} \rightarrow A$  is complete on its own iff it is normalized:  $\langle \psi | \psi \rangle = 1$ .
- (c) A set of costates  $\{\chi_k : A \rightarrow \mathbf{1}\}_k$  is complete if the corresponding states form an orthonormal basis for  $A$ :  $\sum_k |\chi_k\rangle\langle\chi_k| = 1_A$ . In this case the set of costates corresponds to a projective measurement in this basis.
- (d) If  $\{f_i\}_i \subset \text{hom}_{\text{QC}}(A, B)$  and  $\{g_j\}_j \subset \text{hom}_{\text{QC}}(C, D)$  are complete sets of morphisms, the tensor product set  $\{f_i \otimes g_j\}_{ij}$  is also complete.
- (e) If  $\{f_i\}_i \subset \text{hom}_{\text{QC}}(A, B)$  and  $\{g_j\}_j \subset \text{hom}_{\text{QC}}(B, C)$  are complete sets of morphisms, the composited set  $\{g_j \circ f_i\}_{ij}$  is also complete.

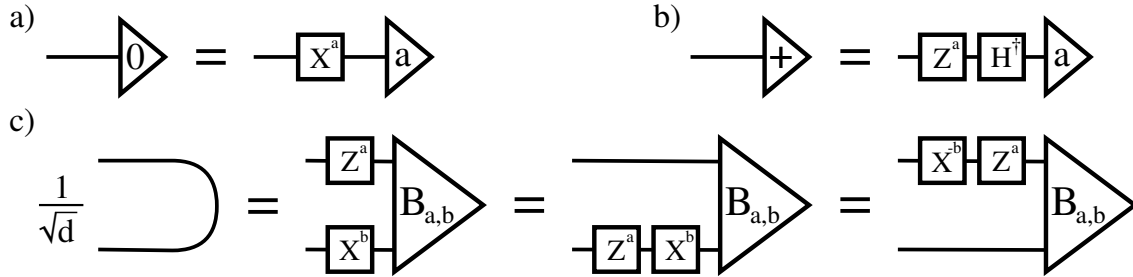


FIG. 17. Representations of (a, b) certain costates and (c) caps in terms of complete sets of costates with local corrections. The generalized Bell costates (labeled with  $B$ ) can be presented in terms of computational basis costates e.g. using the inverse of the circuit in Fig. 3.

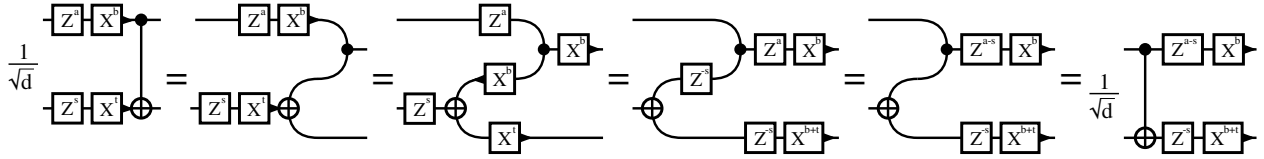
In constructing complete sets of QC-morphisms it is useful to be able to implement caps and certain other costates in terms of projective measurements followed by local unitary corrections dependent on the outcome. This can be done by first expressing the costate in terms of a complete set of standard basis costates (as shown in Fig. 17) and then using Theorem 21 together with commutation rules between various circuit elements and the  $Z$  and  $X$  gates. In the computational basis  $Z^T = Z$  and  $X^T = X^{-1}$ , so they both can readily be slid around caps and caps. By shuttling them along the circuit to positions which causally follow the costate that introduced them (if possible!), the circuit becomes physically implementable. Examples on how this is accomplished in practice are given in the next section.

## IV. APPLICATIONS

Here we present some applications of the extended quantum circuit diagram methods derived in the last section. First we show some examples of circuit simplification, and then derive several well-known quantum protocols for systems of arbitrary dimension using almost no algebra beyond what is implicit in the diagrams.

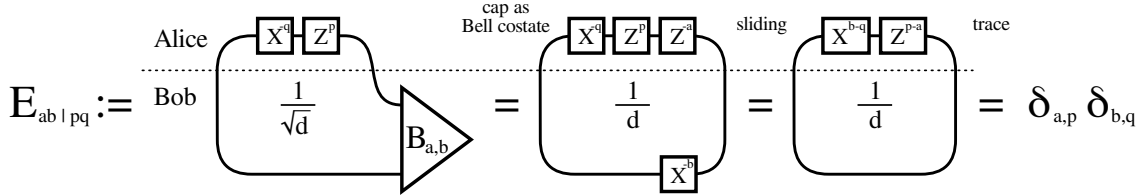
### A. Circuit simplification

**Example 40** (Commuting  $Z$  and  $X$  gates through a NADD gate). Start by breaking the NADD gate into a copy dot and a plus dot. Then apply the commutation rules presented in Fig. 15 to commute the  $Z$  and  $X$  gates through the dots, and finally put the NADD gate together again. The result is the  $d$ -dimensional generalization of the familiar commutation rules between  $\sigma_z$ ,  $\sigma_x$  and a CNOT.



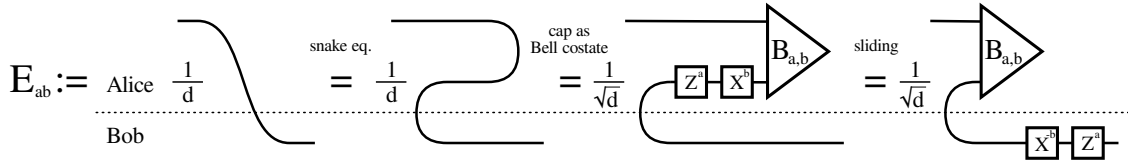
### B. Quantum protocols

**Example 41** (Superdense coding). We start with a diagram representing a cup state followed by local operation  $(p, q)$  by Alice, and finally a Bell measurement with the outcome  $(a, b)$  by Bob. We then express the Bell costate using a cap and  $Z$  and  $X$  gates, slide the gates around the bends and obtain a trace expression which is easily evaluated using Eq. (16).



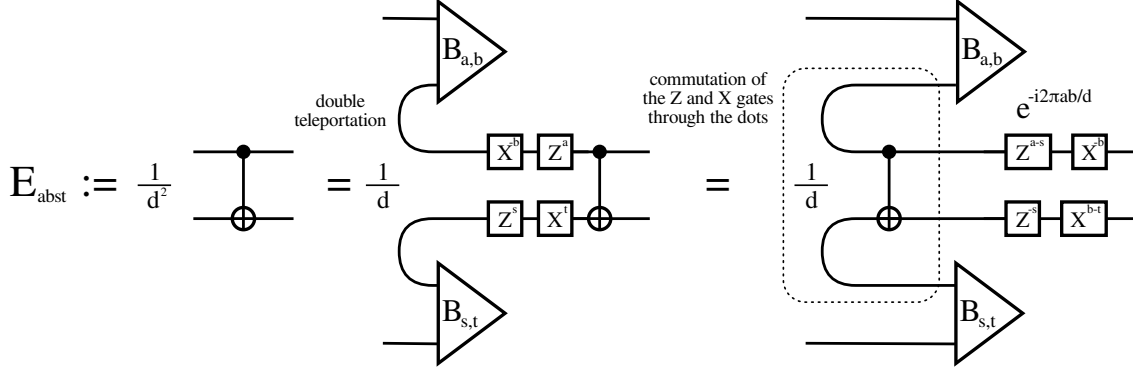
The corresponding Kraus operators are  $E_{ab|pq} = \delta_{a,p} \delta_{b,q}$ . This set of morphisms is complete for all possible local operations  $(p, q)$ . Furthermore, the probability of Bob obtaining the measurement outcome  $(a, b)$  is  $P_{ab} = \text{Tr}(E_{ab|pq} \rho E_{ab|pq}^\dagger) = \delta_{a,p} \delta_{b,q} \text{Tr}(\rho) = \delta_{a,p} \delta_{b,q}$ . Hence the result of Bob's measurement is completely determined by Alice, and she use this protocol to can transmit two d-its worth of information to Bob.

**Example 42** (Teleportation [10]). Using the snake equation, expressing the cap in terms of a Bell costate preceded by  $Z$  and  $X$  gates, and sliding the gates around the cup, we obtain a causal diagram that represents the  $(a, b)$  outcome of a Bell measurement by Alice, followed by local corrections dependent on the measurement result by Bob.



The corresponding Kraus operators are  $E_{ab} = \frac{1}{d} \mathbb{1}$  for all  $a, b$ . This set of morphisms is easily seen to be complete. Hence together these diagrams must represent a physical operation,  $\rho \mapsto \sum_{ab} E_{ab} \rho E_{ab}^\dagger = \rho$ , which faithfully transports any quantum state  $\rho$  from Alice to Bob.

**Example 43** (Teleportation through a gate [24]). Starting from a two-qudit gate (NADD in our example case), we use the above teleportation protocol once for each input qudit, commute the local  $Z$  and  $X$  corrections through the NADD as in Example 40, and finally regroup the gates.



The resulting diagrams each correspond to the same NADD gate operation and form a complete set. This allows us to implement any gate  $U$  in an atemporal order: First we apply the gate to a number of cup states, obtaining the state  $|\tilde{U}\rangle$ , isomorphic to  $U$ . The inputs are then teleported “through” the gate-state, effectively applying  $U$  on them, even if they did not even exist yet when the gate was actually used. Furthermore, the states  $|\tilde{U}\rangle$  (inside the dotted line in the diagram) can be prepared beforehand in large numbers and used only when needed. This is useful e.g. in the case where the success of an individual  $U$  operation is not guaranteed, but the computation itself must not fail.

## V. SUMMARY

Several of the results which were presented extend the state of the art in diagrammatic methods applied to physics. This was accomplished by providing a representation of dagger compact closed categories onto quantum circuit diagrams. Using the corresponding string diagram calculus, the language of quantum circuit diagrams was extended in a way that enables powerful new ways of manipulating and simplifying circuits, while remaining within a framework that is directly and easily applicable to problems stated in the language of quantum information science. We hope the present paper will lead to many new research directions in quantum information science, for both physicists and those working in applied mathematics.

## ACKNOWLEDGMENTS

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## Appendix A: On dualities

Assume we have vector space  $V$  over the field  $\mathbb{K}$ . The *dual space*  $V^*$  is the vector space of linear functionals on  $V$ , that is,  $V^* = \{f : V \rightarrow \mathbb{K}\}$ .

There is a natural isomorphism  $\omega$  between  $V$  and its double dual:

$$\omega : V \rightarrow V^{**}, \quad (\omega(v))(\phi) = \phi(v) \quad \forall v \in V, \phi \in V^*. \quad (\text{A1})$$

Assume we have vector spaces  $A$  and  $B$ , and a linear operator  $O : A \rightarrow B$ . The *transpose*  $O^T : B^* \rightarrow A^*$  of a linear operator is defined by

$$O^T \beta = \beta \circ O \quad \forall \beta \in B^*. \quad (\text{A2})$$

If  $A$  and  $B$  and their duals are given bases  $\{\hat{a}_i \in A\}_i, \{\hat{b}_i \in B\}_i$  and  $\{\tilde{a}_i \in A^*\}_i, \{\tilde{b}_i \in B^*\}_i$ , and these are each others' dual bases, i.e.,  $\tilde{a}_i(\hat{a}_j) = \delta_{ij}, \tilde{b}_i(\hat{b}_j) = \delta_{ij}$ , we can write a matrix representation for  $O$ :

$$O(\hat{a}_j) = \sum_i o_{ij} \hat{b}_i. \quad (\text{A3})$$

This gives us

$$(O^T(\tilde{b}_k))(\hat{a}_j) = \tilde{b}_k(O(\hat{a}_j)) = \sum_i o_{ij} \tilde{b}_k(\hat{b}_i) = o_{kj} = \sum_i o_{ki} \tilde{a}_i(\hat{a}_j) = (\sum_i o_{ki} \tilde{a}_i)(\hat{a}_j). \quad (\text{A4})$$

Hence we have

$$O^T(\tilde{b}_j) = \sum_i o_{ji} \tilde{a}_i = \sum_i o_{ij}^T \tilde{a}_i, \quad (\text{A5})$$

which means the matrix representation of  $O^T$  is given by the matrix transpose of the matrix representation of  $O$ .

Assume we have inner product spaces  $A$  and  $B$ , and a linear operator  $O : A \rightarrow B$ . The *adjoint operator*  $O^\dagger : B \rightarrow A$  is defined by

$$\langle b | Oa \rangle_B = \langle O^\dagger b | a \rangle_A \quad \forall a \in A, b \in B. \quad (\text{A6})$$

**Definition 44** (Conjugate space). The (formal) complex conjugate of a complex vector space  $V$ , is the complex vector space  $\overline{V}$  consisting of all formal complex conjugates of elements of  $V$ . That is,  $\overline{V}$  is a vector space whose elements are in one-to-one correspondence with the elements of  $V$ :

$$\overline{V} = \{\overline{v} \mid v \in V\}, \quad (\text{A7})$$

with the following rules for addition and scalar multiplication:

$$\overline{v} + \overline{w} = \overline{v + w} \quad \text{and} \quad \alpha \overline{v} = \overline{\alpha v}. \quad (\text{A8})$$

Here  $v$  and  $w$  are vectors in  $V$ ,  $\alpha$  is a complex number, and  $\overline{\alpha}$  denotes the complex conjugate of  $\alpha$ .

**Remark 45.** In the case where  $V$  is a linear subspace of  $\mathbb{C}^n$ , the formal complex conjugate  $\overline{V}$  is naturally isomorphic to the actual complex conjugate subspace of  $V$  in  $\mathbb{C}^n$ .

**Remark 46** (Antilinear maps). If  $V$  and  $W$  are complex vector spaces, a function  $f : V \rightarrow W$  is antilinear if

$$f(v + v') = f(v) + f(v') \quad \text{and} \quad f(\alpha v) = \overline{\alpha} f(v) \quad (\text{A9})$$

for all  $v, v' \in V$  and  $\alpha \in \mathbb{C}$ .

One reason to consider the vector space  $\overline{V}$  is that it makes antilinear maps into linear maps. Specifically, if  $f : V \rightarrow W$ , is an antilinear map, then the corresponding map  $\overline{V} \rightarrow W$  defined by

$$\overline{v} \mapsto f(v) \quad (\text{A10})$$

is linear. Conversely, any linear map defined on  $\overline{V}$  gives rise to an antilinear map on  $V$ .

One way of thinking about this correspondence is that the map  $C : V \rightarrow \overline{V}$  defined by

$$C(v) = \overline{v} \quad (\text{A11})$$

is an antilinear bijection. Thus if  $f : \overline{V} \rightarrow W$  is linear, then composition  $f \circ C : V \rightarrow W$  is antilinear, and vice versa.

**Definition 47** (Conjugate linear maps). Any linear map  $f : V \rightarrow W$  induces a conjugate linear map  $\overline{f} : \overline{V} \rightarrow \overline{W}$ , defined by the formula

$$\overline{f}(\overline{v}) = \overline{f(v)}. \quad (\text{A12})$$

The conjugate linear map  $\overline{f}$  is linear. Moreover, the identity map on  $V$  induces the identity map  $\overline{V}$ , and

$$\overline{f} \circ \overline{g} = \overline{f \circ g} \quad (\text{A13})$$

for any two linear maps  $f$  and  $g$ . Therefore, the rules  $V \mapsto \overline{V}$  and  $f \mapsto \overline{f}$  define a functor from the category of complex vector spaces to itself.

If  $V$  and  $W$  are finite-dimensional and the map  $f$  is described by the complex matrix  $A$  with respect to the bases  $\mathcal{B}$  of  $V$  and  $\mathcal{C}$  of  $W$ , then the map  $\overline{f}$  is described by the complex conjugate of  $A$  with respect to the bases  $\overline{\mathcal{B}}$  of  $\overline{V}$  and  $\overline{\mathcal{C}}$  of  $\overline{W}$ .

**Example 48** (Structure of the conjugate). The vector spaces  $V$  and  $\overline{V}$  have the same dimension over the complex numbers and are therefore isomorphic as complex vector spaces. However, there is no natural isomorphism from  $V$  to  $\overline{V}$ . (The map  $C$  is not an isomorphism, since it is antilinear.) The double conjugate  $\overline{\overline{V}}$  is naturally isomorphic to  $V$ , with the isomorphism  $\overline{\overline{V}} \rightarrow V$  defined by

$$\overline{\overline{v}} \mapsto v. \quad (\text{A14})$$

Usually the double conjugate of  $V$  is simply identified with  $V$ .

**Remark 49** (Canonical Isomorphisms). A motivating example is the distinction between a finite-dimensional vector space  $V$  and its dual space  $V^* = \{\phi : V \rightarrow K\}$  of linear maps from  $V$  to its field of scalars  $K$ . These spaces have the same dimension, and thus are isomorphic as abstract vector spaces (since algebraically, vector spaces are classified by dimension, just as sets are classified by cardinality), but there is no "natural" choice of isomorphism  $V \xrightarrow{\sim} V^*$ . If one chooses a basis for  $V$ , then this yields an isomorphism: For all  $u, v \in V$ ,

$$v \xrightarrow{\sim} \phi_v \in V^* \quad \text{such that} \quad \phi_v(u) = v^T u. \quad (\text{A15})$$

This corresponds to transforming a column vector (element of  $V$ ) to a row vector (element of  $V^*$ ) by transpose, but a different choice of basis gives a different isomorphism: the isomorphism "depends on the choice of basis". More subtly, there is a map from a vector space  $V$  to its double dual  $V^{**} = \{x : V^* \rightarrow K\}$  that does not depend on the choice of basis: For all  $v \in V, \phi \in V^*$ ,

$$v \xrightarrow{\sim} x_v \in V^{**} \quad \text{such that} \quad x_v(\phi) = \phi(v). \quad (\text{A16})$$

This leads to a third notion, that of a natural isomorphism: while  $V$  and  $V^{**}$  are different sets, there is a "natural" choice of isomorphism between them. This intuitive notion of "an isomorphism that does not depend on an arbitrary choice" is formalized in the notion of a natural transformation; briefly, that one may consistently identify, or more generally map from, a vector space to its double dual,  $V \xrightarrow{\sim} V^{**}$ , for any vector space in a consistent way. Formalizing this intuition is a motivation for the development of category theory.

**Remark 50** (Notation: natural vs. unnatural isomorphisms). If one wishes to draw a distinction between an arbitrary isomorphism (one that depends on a choice) and a natural isomorphism (one that can be done consistently), one may write  $\approx$  for an unnatural isomorphism and  $\cong$  for a natural isomorphism, as in  $V \approx V^*$  and  $V \cong V^{**}$ . This convention is not universally followed, and authors who wish to distinguish between unnatural isomorphisms and natural isomorphisms will generally explicitly state the distinction.

## Appendix B: Measurements with postselection

Given the state operator  $\rho (= |\psi\rangle\langle\psi|)$  and a set of Kraus operators  $\{E_k\}_k$  which is complete, i.e.  $\sum_k E_k^\dagger E_k = \mathbb{1}$ , the probability of outcome  $k$  is

$$P_k = \text{Tr} \left( E_k \rho E_k^\dagger \right) = \text{Tr} \left( E_k |\psi\rangle\langle\psi| E_k^\dagger \right) = \langle\psi| E_k^\dagger E_k |\psi\rangle = |E_k |\psi\rangle|^2 \quad (\text{B1})$$

and the state after the operation is

$$\begin{aligned} \rho' &= \frac{E_k \rho E_k^\dagger}{P_k} = \frac{E_k |\psi\rangle\langle\psi| E_k^\dagger}{P_k} \\ |\psi'\rangle &= \frac{E_k |\psi\rangle}{|E_k |\psi\rangle|} \end{aligned}$$

Now assume that  $E_k$  is a projector, i.e.  $E_k^\dagger = E_k$  and  $E_k^2 = E_k$ , and given as a sum of orthogonal rank-1 projectors:  $E_k = \sum_i |\phi_i\rangle\langle\phi_i|$ . This gives

$$P_k = \sum_i \langle\phi_i|\rho|\phi_i\rangle = \sum_i |\langle\phi_i|\psi\rangle|^2 \quad (\text{B2})$$

and

$$\rho' = \frac{E_k \rho E_k^\dagger}{P_k}$$

$$|\psi'\rangle = \frac{\sum_i |\phi_i\rangle\langle\phi_i|\psi\rangle}{\sqrt{\sum_i |\langle\phi_i|\psi\rangle|^2}}$$

### Appendix C: Uniqueness of the cup state

Assume we have a bipartite state

$$|\psi\rangle = c_{xy}|x\rangle_A|y\rangle_B \quad (\text{C1})$$

that should play the role of  $|\cup\rangle$ , where the complex coefficients  $c_{xy}$  can be interpreted as elements of the matrix  $C$ . The normalization condition gives

$$\langle\psi|\psi\rangle = c_{xy}^* c_{xy} = \text{Tr}(C^\dagger C) = 1. \quad (\text{C2})$$

We require that  $|\psi\rangle$  should have the following property: For every linear operation

$$f : A \rightarrow A', \quad f = f_{ij}|i\rangle_{A'}\langle j|_A$$

there is another linear operation

$$g^T : B \rightarrow B', \quad g^T = (g^T)_{ij}|i\rangle_{B'}\langle j|_B$$

and vice versa such that the graphical equality in Fig. 18 holds; we want to be able to “slide” the operations around the cup.

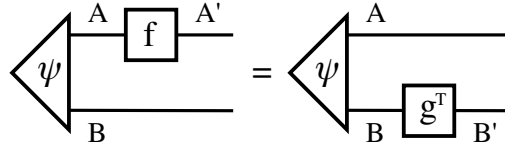


FIG. 18. “Sliding” linear operations around a cup state.

In equation form this is

$$\begin{aligned} f_{ij}c_{xy}|i\rangle_{A'}\langle j|_A|y\rangle_B &= f_{ij}c_{jy}|i\rangle_{A'}|y\rangle_B = f_{ij}c_{jk}|i\rangle_{A'}|k\rangle_B \\ &= (g^T)_{ij}c_{xy}|i\rangle_{B'}\langle j|_B|x\rangle_A = c_{xj}(g^T)_{ij}|x\rangle_A|i\rangle_{B'} = c_{ij}(g^T)_{kj}|i\rangle_A|k\rangle_{B'} \end{aligned} \quad (\text{C3})$$

For the sliding operation to make sense, the dimensions of the external legs must remain the same:  $A' \cong A$ ,  $B' \cong B$ . Thus we have

$$f_{ij}c_{jk} = c_{ij}(g^T)_{kj} = c_{ij}g_{jk} \quad \text{or in matrix form} \quad FC = CG. \quad (\text{C4})$$

Now let us do a singular value decomposition:  $C = U_c \Sigma_c V_c^\dagger$  where  $U_c$  and  $V_c^\dagger$  are unitary and  $\Sigma_c$  is a  $\dim A \times \dim B$  diagonal matrix with the singular values  $\sigma_k$  of  $C$  on the diagonal in descending order. The state normalization condition is equivalent to  $\sum_k \sigma_k^2 = 1$ . We obtain

$$\begin{aligned} F(U_c \Sigma_c V_c^\dagger) &= (U_c \Sigma_c V_c^\dagger)G \\ \Leftrightarrow (U_c^\dagger F U_c) \Sigma_c &= \Sigma_c (V_c^\dagger G V_c) \\ \Leftrightarrow \tilde{F} \Sigma_c &= \Sigma_c \tilde{G}. \end{aligned} \quad (\text{C5})$$

Now, we always have  $\sigma_1 > 0$ . If  $\Sigma_c$  is not square, there are either matrices  $F$  for which there is no  $G$  such that Eq. (C4) holds, or vice versa. Hence we must have  $A \cong B$  as well. In a similar fashion we must also have  $\sigma_k \neq 0 \forall k$ , which means  $\Sigma_c$  is invertible. We obtain

$$\tilde{G} = \Sigma_c^{-1} \tilde{F} \Sigma_c \Leftrightarrow G = C^{-1} F C. \quad (C6)$$

Now assume we wish to impose one additional constraint: The cup state has to map unitary operations to unitary operations. For all unitary matrices  $\tilde{F}$ , we must have

$$\begin{aligned} \tilde{G} \tilde{G}^\dagger &= \Sigma_c^{-1} \tilde{F} \Sigma_c \Sigma_c^\dagger \tilde{F}^\dagger (\Sigma_c^{-1})^\dagger = \Sigma_c^{-1} \tilde{F} \Sigma_c^2 \tilde{F}^\dagger \Sigma_c^{-1} = \mathbb{1} \\ \Leftrightarrow \tilde{F} \Sigma_c^2 &= \Sigma_c^2 \tilde{F}, \end{aligned} \quad (C7)$$

or  $\Sigma_c^2$  must commute with every unitary matrix  $\tilde{F}$ . Now Schur's Lemma for unitary reps of Lie groups says that  $\Sigma_c^2$  and thus  $\Sigma_c$  must be a scalar multiple of identity and thus is completely fixed:  $\Sigma_c = \frac{1}{\sqrt{d}} \mathbb{1}$ , where  $d := \dim A$ .

$$|\psi\rangle = U_{cxi} \Sigma_{ij} V_{c\, jy}^\dagger |x\rangle_A |y\rangle_B = \frac{1}{\sqrt{d}} U_{cxi} V_{c\, iy}^\dagger |x\rangle_A |y\rangle_B = \frac{1}{\sqrt{d}} U_{cxi} |x\rangle_A V_{c\, iy}^\dagger |y\rangle_B = \frac{1}{\sqrt{d}} |U_i^T\rangle_A |V_i^\dagger\rangle_B. \quad (C8)$$

Hence the most general cup state is a local rotation of  $|\cup\rangle$ .

#### Appendix D: Channel-state duality: Choi-Jamiolkowski isomorphism

Channel-state duality refers to the correspondence between quantum channels and quantum states (described by density matrices). This duality arises at several places in modern quantum theory literature — see e.g. [25, 26]. Let  $H_1$  and  $H_2$  be (finite dimensional) Hilbert spaces. The family of linear operators acting on  $H_i$  will be denoted by  $L(H_i)$ . Consider two quantum systems, indexed by 1 and 2, whose states are density matrices in  $L(H_i)$  respectively. A quantum channel, in the Schrödinger picture, is a completely positive linear map

$$\Phi : L(H_1) \rightarrow L(H_2) \quad (D1)$$

that takes a state of system 1 to a state of system 2. Next we describe the so called *dual state* corresponding to  $\rho_\Phi$ .

Let  $E_{ij}$  denote the matrix unit whose  $ij$ -th entry is 1 and zero elsewhere. The (operator) matrix

$$\rho_\Phi = (\Phi(E_{ij}))_{ij} \in L(H_1) \otimes L(H_2) \quad (D2)$$

is called the Choi matrix of  $\Phi$ . By Choi's theorem on completely positive maps,  $\rho_\Phi$  is completely positive if and only if  $\rho_\Phi$  is positive (semidefinite). One can view  $\rho_\Phi$  as a density matrix, and therefore the state dual to  $\Phi$ .

The duality between channels and states refers to the map

$$\Phi \rightarrow \rho_\Phi, \quad (D3)$$

which is a linear bijection. This map is called the Choi-Jamiolkowski isomorphism.

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