Completeness of Graphical Languages for Mixed States Quantum Mechanics

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Abstract

There exist several graphical languages for quantum information processing, like quantum circuits, ZX-Calculus, ZW-Calculus, etc. Each of these languages forms a †-symmetric monoidal category (†-SMC) and comes with an interpretation functor to the †-SMC of (finite dimension) Hilbert spaces. In the recent years, one of the main achievements of the categorical approach to quantum mechanics has been to provide several equational theories for most of these graphical languages, making them complete for various fragments of pure quantum mechanics.

We address the question of the extension of these languages beyond pure quantum mechanics, in order to reason on mixed states and general quantum operations, i.e. completely positive maps. Intuitively, such an extension relies on the axiomatisation of a *discard* map which allows one to get rid of a quantum system, operation which is not allowed in pure quantum mechanics.

We introduce a new construction, the *discard construction*, which transforms any †-symmetric monoidal category into a symmetric monoidal category equipped with a discard map. Roughly speaking this construction consists in making any isometry causal.

Using this construction we provide an extension for several graphical languages that we prove to be complete for general quantum operations. However this construction fails for some fringe cases like the Clifford+T quantum mechanics, as the category does not have enough isometries.

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1 Introduction

Graphical languages that speak of quantum information can be formalised through the notion of symmetric monoidal categories. Hence, it has a nice graphical representation using string diagrams [41]. Qubits are represented by wires, and morphisms by graphical elements where some wires go in, and some others go out, just as in quantum circuits (which is actually a particular case of symmetric monoidal category), and where these graphical elements can be composed either in sequence (usual composition) or in parallel (tensor product). They usually come with an additional structure, a contravariant functor called dagger.

Examples of graphical languages for quantum mechanics and quantum computing are the quantum circuits and the ZX-Calculus [11]. Some variants of the ZX-calculus have been introduced more recently like the ZW-calculus [26] and the ZH-calculus [6]. All these languages are defined using generators (elementary gates) and come with an interpretation functor which associates to any diagram a pure quantum evolution, i.e. a morphism in the category of Hilbert spaces. Given a graphical language, there are generally several ways to represent a quantum evolution, thus a graphical language is also equipped with an equational theory which allows to transform a diagram into another equivalent diagram. A fundamental property, generally hard to prove, is the completeness of the language: given two diagrams representing the same quantum evolution, one can be turned into the other using only the transformation rules in the theory.

The languages considered have usually been built so as to be able to represent any pure quantum evolution, i.e. any perfectly isolated quantum system which hence does not interact with the environment. In this case, the language is called universal for pure quantum mechanics. The hardness of the completeness problem, as well as constraints given by the complexity to physically achieve some gates, focused the research on some restrictions of the languages. On the one hand, finite presentations for the quantum circuits were shown to be complete for some restrictions – namely Clifford [42], one-qubit Clifford+T [37], two-qubit Clifford+T [43], CNot-dihedral [1] –, however none of these restrictions is universal, nor approximately universal. Regarding the ZX-calculus, completeness results exist for non-universal restrictions of the ZX-Calculus [3, 4, 16, 24], but also for the many-qubit Clifford+T ZX-Calculus [31], which was the first completeness result for an approximately universal fragment of the language. Then complete theories have been introduced for the universal ZX-Calculus [28, 33, 32, 44] and ZW-Calculus [27, 28]. The completeness of the graphical languages for pure quantum mechanics is one of the main achievements of the categorical approach to quantum mechanics, and is the cornerstone for the application of this formalism in many areas of quantum information processing. The ZX-Calculus already proved to be useful for quantum information processing [14] (e.g. measurement-based quantum computing [18, 23, 29], quantum codes [17, 9, 20, 22], circuit optimisation [21], foundations [5, 19] ...). Moreover the ZX-calculus can be concretely used through two softwares: Quantomatic [36] and PyZX [34].

The existence of complete graphical languages beyond pure quantum mechanics for more general, not necessarily pure, quantum evolutions is an open question that we address in the present paper.

While pure quantum evolutions correspond to linear maps over Hilbert spaces, probability distributions over quantum states as well as some quantum evolutions like discarding a quantum system can be represented, following the von Neumann approach, by means of density matrices and completely positive maps. The category of completely positive maps has been already studied [39], and in particular the connections between the pure and the van Neumann approaches is a central question in categorical quantum mechanics. Selinger introduced a construction called CPM to turn a category for pure quantum mechanics into a category for density matrices and completely positive maps [40]. Another approach to relate pure quantum mechanics to the general one is the notion of environment structure [10, 12, 15]. The notion of *purification* is central in the definition of environment structure. The CPM-construction and the environment structure approaches have been proved to be equivalent [12].

In terms of graphical languages, the environment structure approach cannot be used in a straightforward way to extend a graphical language beyond pure quantum mechanics. Roughly speaking the environment structure approach provides second order axioms which associates with any equation on arbitrary (non necessarily pure) evolutions an equivalent equation on pure evolutions. Such a second order axiom cannot be easily handled by a equational theory on diagrams. Regarding the CPM-construction, the main property which has been exploited in [14] is that CPM(**C**) is essentially a subcategory of **C**, thus one can use a graphical language which has been designed for **C** in order to represent morphisms in CPM(**C**): Given a complete graphical language for **C**, we can use a subset of the pure diagrams to represent the evolutions in CPM(**C**). The main caveat of this approach is that this subset is not necessarily closed under the equational theory on pure diagrams, and as a consequence does not provide a complete graphical language for CPM(**C**).

Our contributions. In [30] was shown that the category **CPTPM** of completely positive trace-preserving maps is the universal monoidal category with a terminal unit and a functor from the category of isometries. We build upon this result by introducing a new construction, the *discard construction*, which transforms any †-symmetric monoidal category into a symmetric monoidal category equipped with a discard map. Roughly speaking this construction consists in making any isometry causal. Indeed, in quantum mechanics, the isometries (linear maps U such $U^\dagger \circ U = I$) are known to be causal, i.e. applying U and then discarding the subsystem on which it has been applied is equivalent to discarding the subsystem straightaway. Specifically, the discard construction proceeds as follows: first the discard is added to the subcategory of isometries, making the unit of the tensor a terminal object in this sub-category , as pointed out in [30]. Then the discard construction is obtained as the pushout of the resulting category and the initial one.

We show that the discard construction does not always produce an environment structure for the original category, and thus is not equivalent to the CPM construction. We show that a necessary and sufficient condition for the two constructions to be equivalent is that the initial category has enough isometries. We show that most of the categories usually used in the context of the categorical quantum mechanics, like **FHilb** and **Stab**, do have enough isometries, however **Clifford+T** does not.

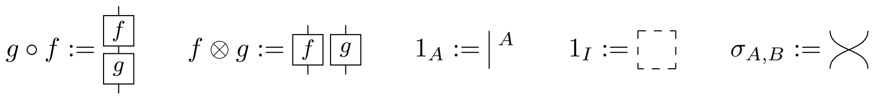
Finally, we show that the discard construction provides a simple recipe to extend graphical languages beyond pure quantum mechanics. We provide an extension for several graphical languages that we prove to be complete for general quantum operations.

Structure of the paper. In section 2, we review some categorical notions used in categorical quantum mechanics. Section 3 is dedicated to the definition of the discard construction and the relation with the CPM construction. Finally, in section 4 we use the discard construction to extend the ZX-calculus to make it complete for general (not necessarily pure) quantum evolutions. The construction is also applied to other graphical languages.

2 Background

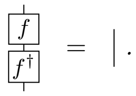
2.1 Dagger symmetric monoidal categories

To avoid any size issue, all our categories are small, the homset of a category $\mathbf{C}$ will be denoted $\mathbf{C}[A, B]$. For simplicity, all the monoidal categories considered in the following will be *strict*. Recall that a *strict symmetric monoidal category* (SMC) $\mathbf{C}$ is a category together with a tensor product bifunctor $\otimes : \mathbf{C} \times \mathbf{C} \to \mathbf{C}$, a unit object I such that $A \otimes I = I \otimes A = A$ and $A \otimes (B \otimes C) = (A \otimes B) \otimes C$, and a symmetry natural isomorphism: $\sigma_{A,B} : A \otimes B \to B \otimes A$ satisfying $\sigma_{A,I} = 1_A$, $\sigma_{A,B\otimes C} = (1_B \otimes \sigma_{A,C}) \circ (\sigma_{A,B} \otimes 1_C)$, and $\sigma_{A,B} \circ \sigma_{B,A} = 1_{B\otimes A}$. A *prop* is an SMC whose set of objects is freely spanned by one object. There is an associated notion of strict symmetric monoidal functor $F : \mathbf{C} \to \mathbf{D}$ which preserves unit, tensors and symmetries. We will use *string diagram* notations for SMC where morphisms are described as boxes and

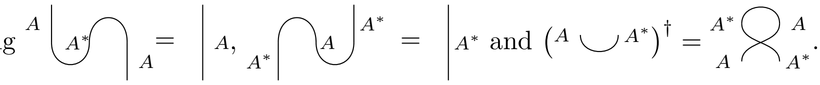


A †-SMC $\mathbf{C}$, is an SMC with an i.o.o. (identity on object) involutive and contravariant SMC-functor $(.)^\dagger : \mathbf{C} \to \mathbf{C}$. That is, every morphism $f : A \to B$ has a dagger $f^\dagger : B \to A$ such that $f^{\dagger\dagger} = f$, moreover the dagger respects the symmetries $\sigma^\dagger_{A,B} = \sigma_{B,A}$. The dagger is a central notion in categorical quantum computing and can be used to define specific properties of morphisms:

▶ **Definition 1.** *$f : A \to B$ is an* isometry *if $f^\dagger \circ f = 1_A$, i.e.*



In this paper most of the categories considered are furthermore compact closed: A dagger compact category (†-CC) is a †-SMC where every object A has a dual object A^* such that for all objects A, there are two morphisms ${}^{A}\cup{}^{A^*} : A \otimes A^* \to I$ and ${}_{A^*}\cap{}_{A} : I \to A^* \otimes A$ satisfying



2.2 Examples

We will consider two kinds of SMCs in this paper: the categories of quantum evolutions and the graphical languages.

Quantum evolutions. Pure quantum evolutions correspond the category of Hilbert spaces. We will consider several of its subcategories: $\mathbf{FHilb}$ is the category of finite dimensional Hilbert spaces whose objects are $\mathbb{C}^n$ and morphisms are linear maps. Its tensor is the usual tensor product of vector spaces and its dagger is the adjoint with respect to the usual scalar product. It is the mathematical model for pure quantum mechanics. In quantum information processing, quantum data is usually carried by qubits, hence $\mathbf{Qubit}$ is the full subcategory of $\mathbf{FHilb}$ with objects of the form $\mathbb{C}^{2^n}$. $\mathbf{Stab}$ is the sub-category of $\mathbf{Qubit}$ which is finitely generated by the Clifford operators: H, S, CNot, the state $|0\rangle$, the projector $\langle 0|$, and the scalar 2 where:

$$\mathrm{H} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \quad \mathrm{S} = \begin{pmatrix}1 & 0\\ 0 & i\end{pmatrix} \quad \mathrm{CNot} = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} \quad |0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \quad \langle 0| = \begin{pmatrix}1 & 0\end{pmatrix}$$

Those are amongst the most commonly used gates in quantum computation (see [38] for details). **Clifford+T** is the same as **Stab** but with the additional generator $T = \left(\begin{smallmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{smallmatrix}\right)$, the morphisms of **Clifford+T** are exactly the matrices with entries in the ring $\mathbb{Z}[i, \frac{1}{\sqrt{2}}]$ [31]. Contrary to **Stab**, **Clifford+T** is *approximately universal* in the sense that $\forall n, m{\in}\mathbb{N}$, $\forall f{\in}\mathbf{Qubit}[\mathbb{C}^{2^n}, \mathbb{C}^{2^m}]$ and $\forall \epsilon{>}0$, there exists $g \in \mathbf{Clifford{+}T}[\mathbb{C}^{2^n}, \mathbb{C}^{2^m}]$ such that $||f-g||{<}\epsilon$. **FHilb**, **Qubit**, **Clifford+T**, and **Stab** are all †-CC. Notice that **Qubit**, **Clifford+T**, and **Stab** are props, but **FHilb** is not.

Probability distributions over pure quantum states as well as some quantum evolutions like discarding a quantum system are not *pure* but can be represented, following the von Neumann approach, by means of density matrices and completely positive maps. Let **CPM** be the category of completely positive maps of finite dimension whose objects are $\mathbb{C}^n$ and $\mathbf{CPM}[\mathbb{C}^n, \mathbb{C}^m] = \{U : \mathbb{C}^{n\times n} \to \mathbb{C}^{m\times m} \mid U \text{ is a completely positive linear map}\}$. Similarly to the pure case, one can define various subcategories of **CPM**. Notice that it can be achieved by the CPM construction described in the next section.

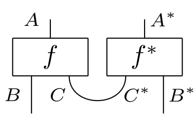
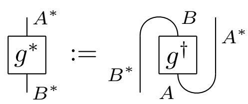
Graphical languages. The second kind of categories we are considering in this paper are graphical languages. They are props which come with interpretation functors defining their semantics. A prop is in fact the equivalent of Lawvere theories for symmetric monoidal theories. They can be presented by generators and relations as one would do for usual theories, see [45] and [7] for a detailed discussion.

▶ **Definition 2.** *A* graphical language $\mathcal{G}$ *is a prop presented by a set of* generators Σ *and a set of* equations E *together with a function* $[\![.]\!] : \Sigma \to \hom(S)$ *called the* interpretation *of* $\mathcal{G}$ *in* S*.* $\mathcal{G}$ *is said to be* sound *if* $[\![.]\!]$ *defines an interpretation functor* $[\![.]\!] : \mathcal{G} \to S$*, and* universal *(resp.* complete*) when this functor is surjective (resp. faithful).*

The ZX-, ZW- and ZH-calculi or the quantum circuits are examples of such categories with semantics in **Qubit**.

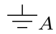
2.3 Environment structures and CPM-construction

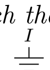
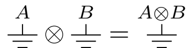
Connecting the Hilbert approach – for pure quantum mechanics – and the von Neumann approach – for open systems – is a central question in categorical quantum mechanics. Selinger pointed out that any †-CC for pure quantum mechanics can be turned into a category for density matrices and completely positive maps via the CPM construction [40]:

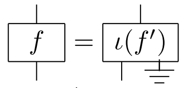
▶ **Definition 3.** *Given a †-CC* $\mathbf{C}$*, let* $\mathrm{CPM}(\mathbf{C})$ *be the †-CC with the same objects as* $\mathbf{C}$ *such that* $\mathrm{CPM}(\mathbf{C})[A,B] = \Bigg\{$  $, f \in \mathbf{C}[A, B\otimes C] \Bigg\}$*, where*  *.*

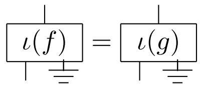
Applying it to **FHilb** one obtains the category **CPM** of completely positives maps. The CPM construction can also be applied to **Qubit**, **Clifford+T**, and **Stab**. Notice that the CPM-construction has been then extended to the non necessarily compact categories [12].

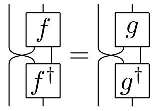
Another approach to relate pure quantum mechanics to the general one is the notion of environment structure [10, 12, 15]. The notion of *purification* is central in the definition of environment structure. Intuitively, it means that (1) there is a discard morphism for every object; (2) any morphism can be purified, i.e. decomposed into a pure morphism followed by a discarding map, and (3) this purification is essentially unique. More formally:

▶ **Definition 4.** *An environment structure for a †-CC* $\mathbf{C}$ *is a CC* $\overline{\mathbf{C}}$ *with the same objects as* $\mathbf{C}$*, an i.o.o SMC-functor* $\iota : \mathbf{C} \to \overline{\mathbf{C}}$ *and for each object* A *a morphism*  $: A \to I$ *such that:*

(1)  $= 1_I$*, and for all* $A, B : \mathbf{C}$*,*  *.*

(2) *For all* $f : A \to B$ *in* $\overline{\mathbf{C}}$*, there is an* $f' : A \to B \otimes X$ *in* $\mathbf{C}$ *such that:* 

(3) *For any* $f : A \to B \otimes X$ *and* $g : A \to B \otimes Y$ *in* $\mathbf{C}$*:* $f \sim_{\text{cp}} g \Leftrightarrow$ 

where the relation $\sim_{\text{cp}}$ *is defined as:* $f \sim_{\text{cp}} g \Leftrightarrow$ 

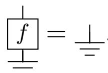
Notice that $\sim_{\text{cp}}$ is technically not a relation on morphisms but on tuples (A, B, X, f) with $f \in \mathbf{C}[A, B \otimes X]$: $(A, B, X, f) \sim_{\text{cp}} (C, D, Y, g)$ if $A = C, B = D$ and f, g satisfy the graphical condition represented above. By abuse of notation, we write $f \sim_{\text{cp}} g$, as the other components of the tuple will be usually obvious from context. We will do the same for our relation $\sim_{\text{iso}}$ below.

CPM is actually an environment structure for the category **FHilb**, and more generally for any †-CC $\mathbf{C}$, CPM($\mathbf{C}$) is an environment structure for $\mathbf{C}$ and conversely any environment structure for $\mathbf{C}$ is equivalent to CPM($\mathbf{C}$) [12]. Actually one can notice that CPM($\mathbf{C}$)$[A, B]$ is nothing but the set of equivalent classes of $\sim_{\text{cp}}$.

The notion of environment structures has also been generalised to the non compact case [12]. We chose here to focus on the compact case.

3 The Discard Construction

We introduce a new construction, the *discard construction*, which consists in adding a discard map for every object of a †-SMC, and thus intuitively transforming a category for pure quantum mechanics into a category for general quantum evolutions.

Causality is a central notion in quantum mechanics which has been axiomatised using a discard map as follows [35]: $f : A \to B$ is *causal* if and only if . Amongst the pure quantum evolutions, the isometries are causal evolutions. The discard construction essentially consists in making any isometry causal. Thus, whereas the CPM construction relies on completely positive maps and the environment structures on the concept of purification, the discard construction relies on causality.

3.1 Definition

We introduce the new construction in three steps. First, given a †-SMC, one can consider its subcategory of isometries:

▶ **Definition 5.** *Given a †-SMC* $\mathbf{C}$*,* $\mathbf{C}_{\text{iso}}$ *is the subcategory with the same objects as* $\mathbf{C}$ *and isometries as morphisms, i.e. for all* $A, B : \mathbf{C}$*,* $\mathbf{C}_{\text{iso}}[A, B] = \{f : \mathbf{C}[A, B], f^\dagger \circ f = 1_A\}$*.*

Notice that $\mathbf{C}_{\text{iso}}$ is an SMC but usually not a †-SMC. Any †-SMC-functor $F : \mathbf{C} \to \mathbf{D}$ between two †-SMC can be restricted to their subcategories of isometries leading to an SMC-functor $F_{\text{iso}} : \mathbf{C}_{\text{iso}} \to \mathbf{D}_{\text{iso}}$. Thus there is a restriction functor iso : †-**SMC** → **SMC**. Remark that this functor preserves fullness and faithfulness. One always has an inclusion i.o.o. faithful SMC-functor: $i_{\text{iso}} : \mathbf{C}_{\text{iso}} \to \mathbf{C}$.

In quantum mechanics, isometries are causal evolutions, i.e. applying an isometry and then discarding all outputs is equivalent to discarding the inputs straight away. As pointed out in [30], adding discard maps to the category of isometries would make I a terminal object. Such a category is said to be *affine symmetric monoidal category* (ASMC). We define the affine completion of an SMC:

▶ **Definition 6.** *Given an SMC* $\mathbf{C}$*, we define* $\mathbf{C}^!$ *as* $\mathbf{C}$ *with an additional morphism* $!_A : A \to I$ *for each object* $A : \mathbf{C}$*. We denote the inclusion functor* $i^! : \mathbf{C} \to \mathbf{C}^!$ *which is strict monoidal and i.o.o. We further impose that* $1_I = \,!_I$*, and that for all* $f : \mathbf{C}[A, B]$*,* $!_B \circ i^!(f) = \,!_A$*. This makes* I *a terminal object in* $\mathbf{C}^!$*, and thus* $\mathbf{C}^!$ *is an ASMC.*

Notice by the way that $!_A \otimes \,!_B = 1_I \circ (\,!_A \otimes \,!_B) = \,!_I \circ (\,!_A \otimes \,!_B) = \,!_{A\otimes B}$. Again given a functor $F : \mathbf{C} \to \mathbf{D}$, one can define a functor $F^! : \mathbf{C}^! \to \mathbf{D}^!$ by $F^!(\,!_A) = \,!_{i^!(F(A))}$ and $F^!(f) = i^!(F(f))$ for the other morphisms. In [30], Huot and Staton show that $\mathbf{CPTPM}$, the category of completely positive trace preserving maps, is equivalent to $\mathbf{FHilb}^!_{\text{iso}}$, thus giving a caracterisation of it via a universal property. We extend this idea to non-trace preserving maps by proceeding to a local affine completion of the subcategory of isometries.

We define the category $\mathbf{C}^{\ground}$ as the pushout of $\mathbf{C}$ and $\mathbf{C}^!_{\text{iso}}$:

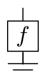
▶ **Definition 7.** *Given a* †*-SMC* $\mathbf{C}$*,* $\mathbf{C}^{\ground}$ *is defined as the pushout in the category of symmetric monoidal categories:*

$$\begin{array}{ccc} \mathbf{C}_{\text{iso}} & \xhookrightarrow{\;i_{\text{iso}}\;} & \mathbf{C} \\ {\scriptstyle i^!}\downarrow & & \downarrow{\scriptstyle \iota_{\mathbf{C}}} \\ \mathbf{C}^!_{\text{iso}} & \xhookrightarrow[\;\iota_{\mathbf{C}^!_{\text{iso}}}\;]{} & \mathbf{C}^{\ground} \end{array}$$

The existence of this pushout follows from the fact that the forgetful functor from strict symmetric monoidal categories to categories $\mathbf{StrictSymMonCat} \to \mathbf{Cat}$ preserves coequalizers, and from [8, Theorem 9.3.9]. As all our functors are i.o.o., we can also describe it simply combinatorially. The objects of $\mathbf{C}^{\ground}$ are the same as $\mathbf{C}$. Its morphisms are equivalence classes generated by formal composition and tensoring of morphisms in $\mathbf{C}^!_{\text{iso}}$ and $\mathbf{C}$. The equivalence relation is generated by the equations of both categories augmented with equations $i^!(f) = i_{\text{iso}}(f)$ for all f in $\mathbf{C}_{\text{iso}}$. The functors $\iota_{\mathbf{C}}$ and $\iota_{\mathbf{C}^!_{\text{iso}}}$ are the natural ways to embed $\mathbf{C}$ and $\mathbf{C}^!_{\text{iso}}$. We will see those formal compositions as string diagrams whose components are morphisms of $\mathbf{C}$ and $\mathbf{C}^!_{\text{iso}}$ wired to each others. Two diagrams represent the same morphism if we can rewrite one into the other applying the equations of both categories and $i^!(f) = i_{\text{iso}}(f)$ for all f in $\mathbf{C}_{\text{iso}}$. This forms a well defined SMC.

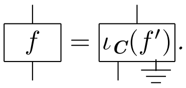
Since the only morphisms in $\mathbf{C}_{\text{iso}}$ which are not identified with the morphisms of $\mathbf{C}$ are those that contain $!_A$, we can see $\mathbf{C}^{\ground}$ as $\mathbf{C}$ augmented with discard maps which delete isometries.

▶ **Definition 8.** *The discard map on an object* A *is defined in* $\mathbf{C}^{\ground}$ *by*  $:= \iota_{\mathbf{C}^!_{\text{iso}}}(\,!_A)$*.*

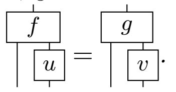
Notice, that for any isometry $f : A \to B$ in $\mathbf{C}^{\ground}$,  $=$ , thus any isometry is causal.

3.2 Relation to environment structures and CPM

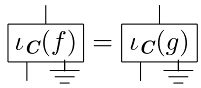
In order to compare the $\mathbf{C}^{\ground}$ construction with environment structures and the CPM construction we need to study in details the purification process in $\mathbf{C}^{\ground}$. First notice that any morphism of $\mathbf{C}^{\ground}$ admits a purification:

▶ **Lemma 9.** *Let* $\mathbf{C}$ *be a* †*-SMC. For all* $f : \mathbf{C}^{\doteqdot}[A, B]$*, there is an* $X : \mathbf{C}$ *and an* $f' : \mathbf{C}[A, B \otimes X]$ *such that* .

The purification needs not be unique, however it satisfies an essential uniqueness condition. To state it we define the relation $\sim_{\text{iso}}$.:

▶ **Definition 10.** *Let* $\mathbf{C}$ *be a* †*-SMC, and two morphisms* $f : A \to B \otimes X$*,* $g : A \to B \otimes Y$*.* $f \sim_{\text{iso}} g$ *if there are two isometries* $u : X \to Z$ *and* $v : Y \to Z$*, such that* .

Notice that the relation $\sim_{\text{iso}}$ is not transitive, thus we consider $\sim^{+}_{\text{iso}}$ its transitive closure to make it an equivalence relation. It is easy to show that if $f \sim^{+}_{\text{iso}} g$ then f and g purify the same morphism of $\mathbf{C}^{\doteqdot}$. The converse is also true:

▶ **Lemma 11.** *For all* $f : A \to B \otimes X$ *and* $g : A \to B \otimes Y$*:* $f \sim^{+}_{\text{iso}} g \Leftrightarrow$ 

So the purification is unique up to $\sim^{+}_{\text{iso}}$. Lemma 11 also gives an alternative definition of $\mathbf{C}^{\doteqdot}$ which relates more easily to the CPM construction. It is the same construction as CPM with $\sim_{\text{cp}}$ replaced by $\sim^{+}_{\text{iso}}$. In other words $\mathbf{C}^{\doteqdot}[A, B]$ is the set of equivalent classes of $\sim^{+}_{\text{iso}}$.

As we have introduced a new discard construction, a natural question is whether $\mathbf{C}^{\doteqdot}$ is an environment structure for $\mathbf{C}$. To be an environment structure, three conditions are required. The first two are satisfied: $\mathbf{C}^{\doteqdot}$ has a discard morphism for every object, and every morphism can be purified. The third one is the uniqueness of the purification: according to the definition of the environment structures, f and g purify the same morphism if and only if $f \sim_{\text{cp}} g$ whereas according to Lemma 11, f and g purify the same morphism if and only if $f \sim^{+}_{\text{iso}} g$. As a consequence $\mathbf{C}^{\doteqdot}$ is an environment structure for $\mathbf{C}$ if and only if $\sim_{\text{cp}} = \sim^{+}_{\text{iso}}$. It turns out that one of the inclusions is always true:

▶ **Lemma 12.** *For any* †*-SMC category* $\mathbf{C}$*, we have* $\sim^{+}_{\text{iso}} \subseteq \sim_{\text{cp}}$*.*

As a consequence, if $\sim_{\text{cp}} \neq \sim^{+}_{\text{iso}}$, it means that there are some morphisms f, g that are equal in $\sim_{\text{cp}}$ but cannot be proved equal in $\sim^{+}_{\text{iso}}$. Intuitively it means the category has not enough isometries to prove those terms equal, which leads to the following definition:

▶ **Definition 13.** *A* †*-SMC category* $\mathbf{C}$ *has* enough isometries *if the equivalences relations* $\sim_{\text{cp}}$ *and* $\sim^{+}_{\text{iso}}$ *of* $\mathbf{C}$ *are equal.*

▶ **Lemma 14.** *Given a* †*-SMC* $\mathbf{C}$*, the following properties are equivalent:*
1. $\mathbf{C}$ *has enough isometries;*
2. $\mathbf{C}^{\doteqdot}$ *is an environment structure for* $\mathbf{C}$*;*
3. $\mathbf{C}^{\doteqdot} \simeq \mathrm{CPM}(\mathbf{C})$.

Notice that if $\mathbf{C}$ has enough isometries, the discard construction provides a definition of $\mathrm{CPM}(\mathbf{C})$ via a universal property. This gives a more direct way to build the environment, avoiding to deal with the equivalence classes of the CPM construction.

▶ Remark 15. Let's focus for a moment on the category $\mathrm{Causal\,CPM}(\mathbf{C})$ of causal maps, that is the subcategory of maps cancelled by the discards in $\mathrm{CPM}(\mathbf{C})$. We have that: $\sim_{\text{cp}} \subseteq \sim^{+}_{\text{iso}} \Rightarrow \mathbf{C}^{!}_{\text{iso}} \simeq \mathrm{Causal\,CPM}(\mathbf{C})$. In fact by Lemma 14, $\mathrm{CPM}(\mathbf{C}) \simeq \mathbf{C}^{\doteqdot}$, and then the subcategory $\mathrm{Causal\,CPM}(\mathbf{C})$ is equivalent to the subcategory of maps cancelled by the discards in $\mathbf{C}^{\doteqdot}$ which is equivalent to $\mathbf{C}^{!}_{\text{iso}}$. $\mathrm{Causal\,CPM}(\mathbf{FHilb})$ being exactly $\mathbf{CPTPM}$, we have recovered the result of [30].

3.3 Examples

We consider the usual subcategories of **FHilb** used for pure quantum mechnanics and show in each case whether the discard construction produces an environment structure or not. First of all, thanks to the Stinespring dilation theorem, $\mathbf{FHilb}^{⏚}$ is not only an environment structure for **FHilb**, but the relation $\sim_{\text{iso}}$ is also transitive in this case:

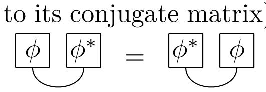
▶ **Proposition 16.** $\mathbf{FHilb}^{⏚}$ *is an environment structure for* **FHilb**. *Furthermore* $\sim_{\text{iso}}^{+} = \sim_{\text{iso}}$.

When dealing with graphical languages we will be more interested in the full subcategory **Qubit** of **FHilb**:

▶ **Proposition 17.** $\mathbf{Qubit}^{⏚}$ *is an environment structure for* **Qubit**.

Notice that in general, the property of having enough isometries does not transfer to full subcategories: If **D** is a full subcategory of **C**, we might have $f \sim_{\text{iso}}^{+} g$ on **C** but $f \not\sim_{\text{iso}}^{+} g$ on **D**. This could happen for two reasons: First the chain of intermediate morphisms that prove that $f \sim_{\text{iso}}^{+} g$ might live outside of **D**. Second, the isometries that "prove" that $f \sim_{\text{iso}}^{+} g$ on **C** might have codomain outside of **D**.

If our category is not a full subcategory, then everything falls apart, and finding conditions that guarantee that $\mathbf{C}^{⏚}$ is an environment structure for **C** is not easy.

For subcategories of **Qubit**, necessary conditions can be given. This category has the peculiarity that $\cdot^*$ is the identity on objects and that $f^{**} = f$ for all morphisms ($\cdot^*$ maps a matrix to its conjugate matrix). In particular, for any state $\phi : I \to I \otimes X$, we have $\phi^* \sim_{\text{cp}} \phi$. Indeed  .

So a necessary condition for a subcategory of **Qubit** to behave nicely is that for all states ϕ, we have $\phi^* \sim_{\text{iso}}^{+} \phi$. This is the case in **Stab**: Given a stabilizer state ϕ, there always exists a stabilizable unitary U s.t. $U\phi = \phi^*$. In fact:

▶ **Proposition 18.** $\mathbf{Stab}^{⏚}$ *is an environment structure for* **Stab**.

The main idea of the proof is to use the map/state duality, and structural results about bipartite stabilizer states [2].

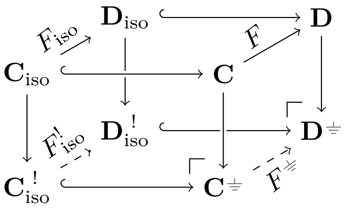
No such unitary exists in general in **Clifford+T**: For almost all states ϕ, there is no unitary U (and actually no morphism at all) s.t. $U\phi = \phi^*$. **Clifford+T** therefore has not got enough isometries:

▶ **Proposition 19.** $(\mathbf{Clifford{+}T})^{⏚}$ *is not an environment structure for* **Clifford+T**. *More precisely, there exists a state* ϕ *s.t.* $\phi \sim_{\text{cp}} \phi^*$ *but* $\phi \not\sim_{\text{iso}}^{+} \phi^*$. *One can take for example* $\phi = 1 + 2i$ *(in this case* ϕ *is a state with no input and outputs, hence a scalar).*

Note that for all categories above, we have $\sim_{\text{iso}}^{+} = \sim_{\text{iso}}$. That it holds in **Qubit** and **FHilb** is a consequence of the Witt extension theorem: Every isometry $f : A \to B$ is equal to a unitary $g : B \to B$ precomposed with a canonical embedding from A to B. It it well known in **Stab** and it is true in **Clifford + T** by [25, Lemma 5].

4 Application to the ZX-Calculus and other graphical languages

We now focus on the behavior of interpretation functors with respect to the discard construction. The discard construction defines a functor $(\_)^{⏚} : \dagger\text{−}\mathbf{SMC} \to \mathbf{SMC}$. Indeed, given a †-SMC functor F, F_{iso} and $F_{\text{iso}}^{!}$ uniquely define a functor $F^{⏚}$ by pushout.



The following lemma and theorem are the main tools to apply the discard construction to graphical languages:

▶ **Lemma 20.** *If F is faithful and if $F_{\text{iso}} : \mathbf{C}_{\text{iso}} \to \mathbf{D}_{\text{iso}}$ is surjective, then $F(f) \sim^{+}_{\text{iso}} F(g) \Rightarrow f \sim^{+}_{\text{iso}} g$.*

▶ **Theorem 21.** *Let $\mathbf{C}$ and $\mathbf{D}$ be two †-SMCs and $F : \mathbf{C} \to \mathbf{D}$ a †-SMC-functor. If F is faithful and if $F_{\text{iso}} : \mathbf{C}_{\text{iso}} \to \mathbf{D}_{\text{iso}}$ is surjective, then $F^{\text{⏚}} : \mathbf{C}^{\text{⏚}} \to \mathbf{D}^{\text{⏚}}$ is faithful. If furthermore F is surjective then $F^{\text{⏚}}$ is surjective and faithful.*

Notice that the hypothesis on F_{iso} is very strong, as it makes it an isomorphism: We want it to be surjective as we do not want to lose even one isometry. In particular we do not know if the theorem still applies if F is merely an equivalence of categories.

Reformulating for graphical languages this gives:

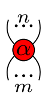
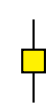
▶ **Corollary 22** (of Theorem 21)**.** *Given a †-CC $\mathbf{C}$ with enough isometries, if $\mathcal{G}$ is a †-CC universal complete graphical language for $\mathbf{C}$ then $\mathcal{G}^{\text{⏚}}$ is a universal complete language for* $\mathrm{CPM}(\mathbf{C})$.

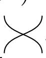
This provides a general recipe. We start with a universal complete graphical language $\mathcal{G}$. We build $\mathcal{G}^{\text{⏚}}$, by Theorem 21, $[\![.]\!]^{\text{⏚}} : \mathcal{G}^{\text{⏚}} \to \mathbf{C}^{\text{⏚}}$ is full and faithful. Furthermore $\mathbf{C}^{\text{⏚}} \simeq \mathrm{CPM}(\mathbf{C})$. $\mathcal{G}^{\text{⏚}}$ as a prop can be presented by adding one new generator ⏚ to the signature Σ and one equation for each isometry of $\mathcal{G}$. In general, if one is provided with a spanning set of the isometries, the number of equations can be drastically reduced. We just need one equation for each element of this set. We then obtain a universal complete graphical language.

We will now briefly review the ZX-calculus and some of its twin languages. They are all universal and complete for subcategories of **Qubit**. Each time we will apply the recipe with a well chosen spanning set and provide the additional axioms involving ⏚. We will not discuss minimality, i.e. if adding these new axioms can help to simplify others.

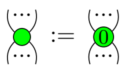
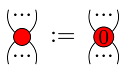
4.1 The ZX-calculus

The ZX-Calculus was introduced in [11] by Coecke and Duncan for pure quantum evolutions. It is a †-compact prop generated by:

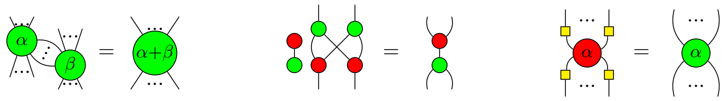
$R_Z^{(n,m)}(\alpha) : n \to m ::$  $R_X^{(n,m)}(\alpha) : n \to m ::$  $H : 1 \to 1 ::$ 

and the two compositions: spacial $(. \otimes .)$ and sequential $(. \circ .)$. The symmetric and compact structure are provided by $\sigma : 2 \to 2 ::$ , $\epsilon : 2 \to 0 ::$  and $\eta : 0 \to 2 ::$ .

To simplify, the red and green nodes are represented empty when holding a 0 angle:

 and 

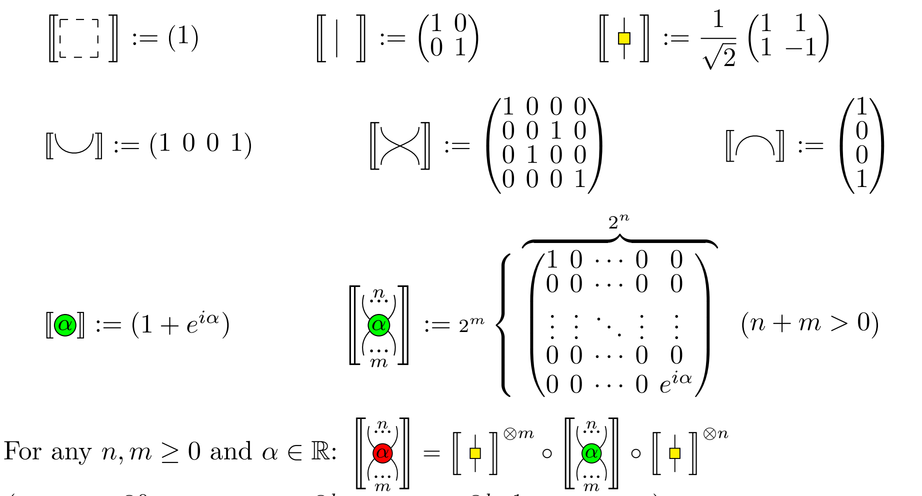
The language is universal [11]. So far, it has two complete axiomatisations [28, 33]. Some of the main axioms are:



ZX-diagrams represent quantum evolutions, so there exists a functor $[\![.]\!] : \mathrm{ZX} \to \mathbf{Qubit}$, called the *standard interpretation*, which associates to any diagram $D : n \to m$ a linear map $[\![D]\!] : \mathbb{C}^{2^n} \to \mathbb{C}^{2^m}$ inductively defined as follows:

$[\![.]\!]$

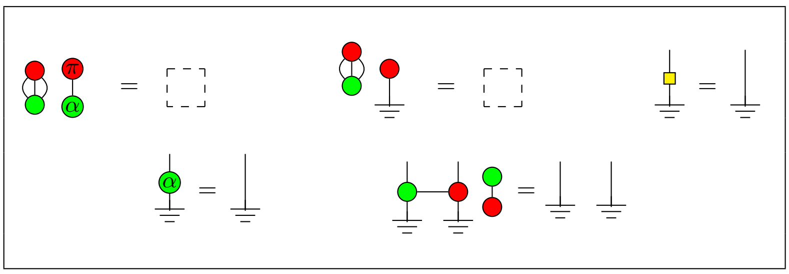
$[\![D_1 \otimes D_2]\!] := [\![D_1]\!] \otimes [\![D_2]\!]$ $\qquad$ $[\![D_2 \circ D_1]\!] := [\![D_2]\!] \circ [\![D_1]\!]$



$\big($where $M^{\otimes 0} = (1)$ and $M^{\otimes k} = M \otimes M^{\otimes k-1}$ for $k \in \mathbb{N}^*\big)$.

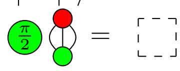
Theorem 21 provides a recipe for transforming the language for mixed states and CPMs. The resulting language ZX$^{\ground}$ can be seen as a prop with the generators of the ZX-Calculus, augmented with $\ground$ and with the axiomatisation enriched with $\{\ground \circ D = \ground \mid D^\dagger \circ D = I\}$. We actually do not need an infinite axiomatisation. Indeed, the set of isometries of the ZX-Calculus can be finitely generated.

Using ($e^{i\alpha}$, $|0\rangle$, H, $R_Z(\alpha)$, CNot) as spanning set of the isometries [38], we obtain only five axioms:



4.2 The $\frac{\pi}{2}$ fragment of ZX-calculus

The ZX$_{\frac{\pi}{2}}$ is obtained from ZX by restricting phases α to $\{0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}\}$. It is universal and complete for **Stab** [3] with the adequate axiomatisation. Moreover according to Lemma 18 **Stab**$^{\ground}$ is an environment structure for **Stab**.

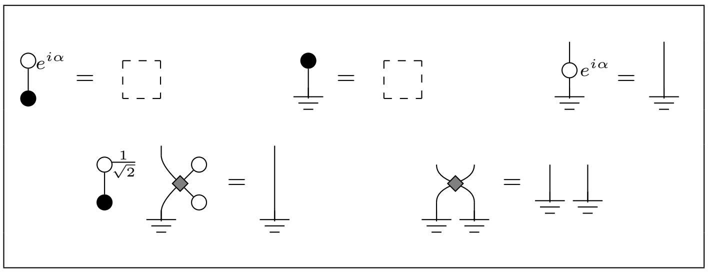
The set ($e^{i\frac{\pi}{4}}$, $|0\rangle$, H, $R_Z(\alpha)$, CNot), with α restricted to multiples of $\frac{\pi}{2}$, is a spanning set of isometries in **Stab** (notice that $e^{i\frac{\pi}{4}} = 2\,\langle 0|\, HSH\, |0\rangle\!\langle 0|\, H\, |0\rangle$ is in **Stab**), so adding the same set of equations than in $\mathrm{ZX}^{\ground}$ with additional rule  will provide a complete axiomatisation for $\mathrm{ZX}^{\ground}_{\frac{\pi}{2}}$.

4.3 The Clifford+T fragment of ZX-calculus

Restricting ZX to angles multiples of $\pi/4$, we obtain a language which is known to be universal and complete for **Clifford+T** [31]. However, as shown by Lemma 19, the semantic category **Clifford+T** does not have enough isometries. The discard construction is strictly coarser than CPM for this fragment. So we leave open the complete axiomatisation of quantum operations for this fragment.

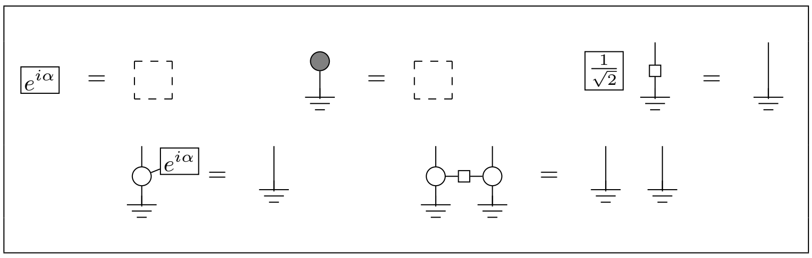
4.4 The ZW-calculus

The ZW-Calculus was introduced in [26], deriving from the GHZ/W-Calculus [13], where the main two generators are two non-equivalent ways to entangle three qubits, the so-called GHZ and W states. The language was made complete for pure quantum mechanics in [28]. Since CNot is hard to express in this calculus, we choose another set of universal diagrams, more suited to ZW, namely ($e^{i\alpha}$, $|1\rangle$, $R_Z(\alpha)$, H, CZ $\circ$ SWAP). The resulting rules for $\mathrm{ZW}^{\ground}$ are:



4.5 The ZH-Calculus

The ZH-Calculus was introduced and proved to be complete in [6]. The point of this language is to easily represent hypergraph-states, a generalisation of graph-states, a useful resource for quantum computing. This language has been specifically designed to easily represent the multi-controlled Z (which constitute the hyperedges in the hypergraph-states). So in particular, CZ and $R_Z(\alpha)$ are easily representable. Up to a scalar, H is also easily doable, and $[\![X^{(0,1)}]\!] = |0\rangle$. Hence, choosing ($e^{i\alpha}$, $|0\rangle$, H, $R_Z(\alpha)$, CZ) as spanning set, we only need the axioms:



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