Completeness of Graphical Languages for Mixed States Quantum Mechanics

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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 [34]. 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 [8]. Some variants of the ZX–calculus have been introduced more recently like the ZW–calculus [21] and the ZH–calculus [5]. 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 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 rep-

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resent 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. Finite presentations for the quantum circuits were shown to be complete for some restrictions - namely Clifford [35], one-qubit Clifford+T [31], two-qubit Clifford+T [36], 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 [2, 3, 12, 20], but also for the many-qubit Clifford+T ZX-Calculus [26], 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 [23, 27, 28, 37] and ZW-Calculus [22, 23]. 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 [10] (e.g. measurement-based quantum computing [14, 19, 24], quantum codes [13, 6, 16, 18], circuit optimisation [17], etc.). Moreover the ZX-calculus can be concretely used through two softwares: Quantomatic [30] and PyZX [29].

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. Selinger introduced a construction called CPM to turn a category for pure quantum mechanics into a category for density matrices and completely positive maps [33]. Another approach to relate pure quantum mechanics to the general one is the notion of environment structure [7, 9, 11]. 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 [9].

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 cannot be easily handled by a equational theory on diagrams. Regarding the CPM-construction, the main property which has been exploited in [10] is that $CPM(\mathbf{C})$ is essentially a subcategory of \mathbf{C} , thus one can use a graphical language which has been designed for \mathbf{C} in order to represent morphisms in $CPM(\mathbf{C})$: Given a complete graphical language for \mathbf{C} , we can use a subset of the pure diagrams to represent the evolutions in $CPM(\mathbf{C})$. 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 $CPM(\mathbf{C})$.

Our contributions. In [25] 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 \dagger -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 [25]. 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.

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