Complete positivity and natural representation of quantum computations

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The referenced article is about semantic models of quantum computation. In common with other approaches to programming language semantics [Win93], the general idea is to interpret a type A as a space $[\![A]\!]$ of observations about A. One interprets a computation $x : A \vdash t : B$, that produces a term t of type B but depends on a term x of type A, as a predicate transformer $[\![B]\!] \to [\![A]\!]$ which maps a predicate on B to its weakest precondition (See e.g. [DP06, Ren13, Cho14]).

In more detail, one interprets a type A as a C*-algebra of operators $[\![A]\!]$, and the computations describe maps between C*-algebras that are in particular *positive*: it is actually only the positive elements of the algebra that describe the observables, and these must be preserved by predicate transformers. In fact, they should be *completely positive*. Informally this means that one can run the computation on a subsystem of a bigger system; for example, we could adjoin an extra qubit to the system and still run the computation. More formally it means that not only does the map $[\![t]\!] : [\![B]\!] \to [\![A]\!]$ preserve positive elements, but also $\mathrm{id}_{[\![\mathrm{qubit}]\!]} \otimes [\![t]\!] : [\![\mathrm{qubit}]\!] \otimes [\![B]\!] \to [\![\mathrm{qubit}]\!] \otimes [\![A]\!]$ preserves positive elements.

The first contribution of this paper is a technique for building representations of quantum computation in terms of completely positive maps. In the second half of the paper we demonstrate our technique by making some first steps in the development of a 'quantum domain theory'.

A technique for building representations. A representation is a full and faithful functor $F : \mathbf{C} \to \mathbf{R}$, that is, a functor for which each function $F_{A,B} : \mathbf{C}(A,B) \to \mathbf{R}(F(A),F(B))$ is a bijection.

From a programming language perspective, where objects interpret types and morphisms interpret programs, a representation gives two things. Firstly, it gives a way of interpreting types as different mathematical structures, which can be illuminating or convenient, while retaining essentially the same range of interpretable programs. Secondly, since the category $\mathbf{R}$ may be bigger than $\mathbf{C}$, it gives the chance to have more structure without altering the interpretation of programs at existing types.

There are several existing representations which allow us to understand and analyze quantum computations in terms of different structures, such as convex sets (e.g. [JWW15]), domains (e.g. [Ren14]), partial monoids and effect algebras (e.g. [Jac12]). However, many of these representations are valid for positive maps but not for completely positive maps, and so they do not fully capture quantum computation.

Our contribution is a general method for extending these representations to completely positive maps, widely accepted as a model of first-order quantum computation (e.g. [Sel04, DP06, Ren14, Cho14, Sta15]).

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The method allows us to convert a full and faithful functor

$$\text{(positive maps)} \longrightarrow \mathbf{R}$$

(where **R** is an arbitrary category) into a full and faithful functor

$$\text{(completely positive maps)} \longrightarrow [\mathbf{N}, \mathbf{R}]$$

where **N** is a category whose objects are natural numbers n and maps $n \to m$ are $n \times m$ complex matrices, composed by matrix multiplication. The category $[\mathbf{N}, \mathbf{R}]$ is the category of functors $(\mathbf{N} \to \mathbf{R})$ and natural transformations between them.

We first consider a functor

$$M : \text{(C*-algebras and completely positive maps)} \to [\mathbf{N}, \text{(C*-algebras and positive maps)}]$$

where $M(A)(n)$ is the C*-algebra of $n \times n$ matrices in A, that is, an entanglement of an n-level quantum system with A.

This will lead us to our first main result:

Theorem. *The functor M is full and faithful: completely positive maps are in natural bijection with families of positive maps.*

(Faithfulness is immediate. Fullness is more involved, since one must show that every natural family of positive maps is completely determined by a single completely positive map.)

As a corollary, we exhibit full and faithful representations of the following forms:

$$\begin{aligned}
\text{(completely positive maps)} &\to [\mathbf{N}, \text{(cones and affine maps)}] \\
\text{(completely positive maps)} &\to [\mathbf{N}, \text{(convex sets and affine maps)}] \\
\text{(completely positive maps)} &\to [\mathbf{N}, \text{(effect modules and effect modules homomorphisms)}]
\end{aligned}$$

Towards a quantum domain theory. In the second part of the paper we demonstrate our technique by making some first steps in the development of a 'quantum domain theory', in which Scott-continuous functions are replaced by Scott-continuous natural transformations. The ultimate goal in this line of work is to analyze all kinds of quantum programming with recursive types by solving domain equations involving qubits. For example, one should expect a solution A to the equation

$$A = (\mathsf{qubit} \overline{\otimes} A)_{\perp}$$

which would be a type of infinite streams of qubits. In this paper we exhibit (for the first time) a domain theory that supports qubits and lifting.

For the reader familiar with semantics of programming languages, we recall basic ideas for the semantics of quantum programming languages in W*-algebras, which are C*-algebras with interesting domain-theoretic properties. A type A is interpreted as a W*-algebra $[\![A]\!]$. A terminating computation-in-context $x_1 : A_1, \ldots, x_n : A_n \vdash t : B$ is interpreted as a completely positive unital map (or CPU-map) $B \to \bigotimes_i A_i$, transforming observations about the result type to observations about the input types.

Let $[\![\mathsf{qubit}]\!] = M_2$, and consider $\mathbb{C}$ be the tensor unit. A computation $\vdash t : \mathsf{qubit}$ that generates a qubit with no inputs is interpreted as a *state*, i.e. a CPU-map $M_2 \to \mathbb{C}$.

We begin with the observation that taking states of a W*-algebra yields a representation of positive maps in terms of affine maps between convex sets. We use this to build a representation

$$\text{(W*-algebras and completely positive maps)} \longrightarrow [\mathbf{N}, \text{(convex sets and affine maps)}]$$

We can now extend the representation with domain theoretic structure, by replacing convex sets with directed complete convex sets. Thus 'quantum domains' are defined to be functors

$$\mathbf{N} \to \text{(convex dcpos and affine continuous maps).}$$

and quantum computations are interpreted as affine Scott-continuous natural transformations between quantum domains. We show that the category of quantum domains supports various constructions, including tensor with quantum data and lifting.

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