A process theory of pure quantum maps

Summary.
(1) From linear maps to quantum maps.
(2) The theory of pure quantum maps.

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Introduction.

The process theory of linear maps is enough to represent typical primitives in quantum computation as processes. For example, classical logic gates are made into linear maps as follows[1].

For example,

Encoding such gates as linear maps is key to the circuit model of quantum computation, namely when restricting to gates that yield unitary linear maps, such as NOT. Typical quantum gates, such as CNOT, are expressed similarly
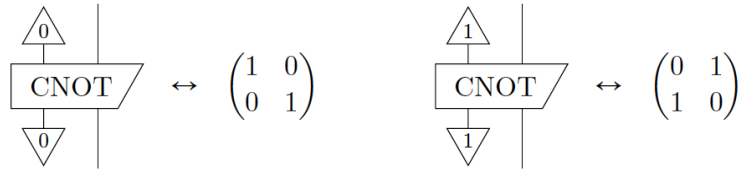

whose matrix representation

$$
\begin{matrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
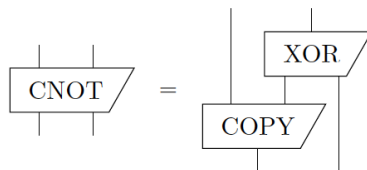0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{matrix}
$$

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[1] Pictures are taken from Coecke and Kissinger book, *Picturing Quantum processes*, CUP, 2017.

is properly explained by the fact that the first basis element selecting which transformation should be applied to the second, as depicted below.
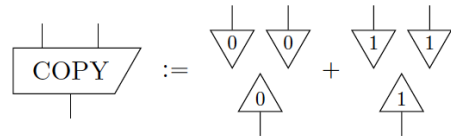
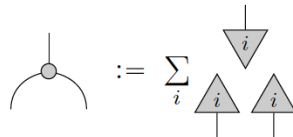$$\text{CNOT}\langle 0,0 \rangle \quad \leftrightarrow \quad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \text{CNOT}\langle 1,1 \rangle \quad \leftrightarrow \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Exercise 1

Show that

$$\text{CNOT} \quad = \quad \text{XOR} \circ \text{COPY}$$

where

$$\text{COPY} \quad := \quad \langle 0 | 0 \rangle \langle 0 | + \langle 1 | 1 \rangle \langle 1 |$$

The XOR gate is, up to a scalar, the adjoint of COPY over the Hadamard basis

$$|+\rangle := \tfrac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle \right) \qquad |-\rangle := \tfrac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle \right)$$

which in the diagrammatic language ZX-calculus[2] is depicted as

$$\bigcirc \quad := \quad \sum_i \ \overset{i}{\triangledown}\ \triangle_i\ \triangle_i$$

Actually,

$$\overset{k}{\triangle}\underset{i\ \ j}{\bigcirc} \ = \ \left(\begin{array}{c} \overset{k}{\triangle} \\ \overset{0}{\triangle} \\ \underset{i\ \ j}{\triangle_0\ \triangle_0} \end{array} + \begin{array}{c} \overset{k}{\triangle} \\ \overset{1}{\triangle} \\ \underset{i\ \ j}{\triangle_1\ \triangle_1} \end{array} \right) \ = \ \frac{1}{\sqrt{2}}\cdot\frac{1}{2}\left(1 + (-1)^{i+j+k} \right)$$

---

[2]The name comes from the Z and X basis, i.e. the computational and the Hadamard bases.

because

$$
\begin{array}{ccccc}
\text{} & = & \text{} & = & \dfrac{1}{\sqrt{2}}
\end{array}
\qquad
\begin{array}{ccccc}
\text{} & = & \text{} & = & (-1)^{i}\dfrac{1}{\sqrt{2}}
\end{array}
$$

Expression

$$
\frac{1}{\sqrt{2}}\cdot\frac{1}{2}\left(1+(-1)^{i+j+k}\right)
$$

is equal to $\frac{1}{\sqrt{2}}$ if $i+j+k$ is even, and 0 otherwise. But $i+j+k$ is even when $i \, \mathsf{XOR} \, j = k$. Thus, ignoring factor $\frac{1}{\sqrt{2}}$, this corresponds to XOR.

Similarly, the Hadamard gate, which maps the Hadamard basis into the computational one is the self-conjugated, self-adjoint linear map

$$
\boxed{H} \;\; := \;\; \sum_{i} \;\; \text{}
$$

Exercise 2

Show that

$$
\text{} \quad := \quad \tfrac{1}{\sqrt{2}}\left(\text{} + \text{} \right)
$$

$$
\text{} \quad := \quad \tfrac{1}{\sqrt{2}}\left(\text{} + \text{} \right)
$$

$$
\text{} \quad := \quad \tfrac{1}{\sqrt{2}}\left(\text{} - \text{} \right)
$$

$$
\text{} \quad := \quad \tfrac{1}{\sqrt{2}}\left(\text{} - \text{} \right)
$$

forms a basis for $\mathbb{C}^2 \otimes \mathbb{C}^2$ which does not correspond to a product of two bases for $\mathbb{C}^2$.

Linear maps, however, are not full adequate to represent quantum processes. For example, quantum processes are blind to global phases as they are not detected by quantum measurements. On the other hand, composing a state and an effect yields a scalar which in the theory of linear maps is a complex number, and not a probability as expected by the generalised Born rule. Both these issues are solved by a curious, but straightforward procedure: process doubling.

Process doubling.

Multiplying a scalar by its conjugate, if its state and effect components are both normalised, yields a real number in the interval $[0, 1]$, i.e. a probability. This means that any normalised state along with any orthonormal basis yields a probability distribution, considering *doubled* inner products.
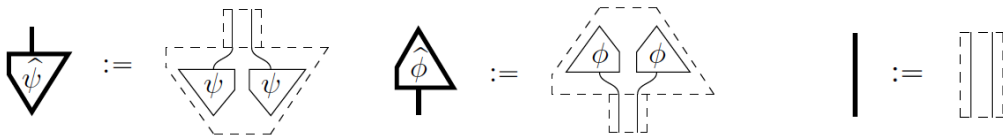

(mirrored) copy 2   copy 1
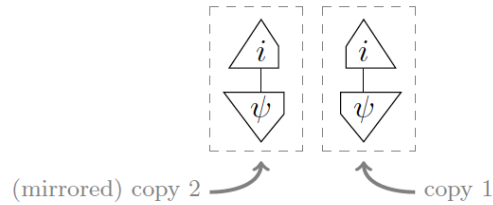
Exercise 3

Verify that

$$\sum_i \ \triangle\!\!\triangle = 1$$

Doubling states and processes amounts to define for each state ϕ of type A its doubled version $\hat{\phi}$ of type $\hat{A}$. A new, bold notation is used to simplify the diagrams as follows.

Exercise 4

The doubling procedure is related to the passage from a pure state vector $|\phi\rangle$ to the corresponding density operator which typically plays the role of a quantum state in the usual approaches to quantum computation. Explain why.

Another advantage of the doubling procedure is to eliminate global phases. Indeed, two states become the same state when doubled if and only if they are equal up to some number

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$e^{i\alpha}$ for $\alpha \in [0, 2\pi[$, i.e.

The doubling procedure extends to processes in the obvious way

Care is needed when dealing with processes with several inputs/outputs: pins must be connected in order and taking into consideration that the conjugate of a process is pictured as its mirror image — so, inputs and outputs are counted from right-to-left rather than left-to-right, which introduces a 'twist' in the wires connected to the conjugate process.

This procedure yields a theory of doubled processes which will be referred to in the sequel as *pure quantum maps*. As a process theory this is simply a sutbheory of linear maps built as follows: its types are $\hat{A}$ for all Hilbert spaces A, and its processes are $\hat{f} : \hat{A} \longrightarrow \hat{B}$ for all linear maps $f : A \longrightarrow B$. Being a subtheory of linear maps, pure quantum maps admits string diagrams. In particular,

and

Exercise 5

Verify the yanking laws in the theory of pure quantum maps.

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Exercise 6

Show that doubling preserves sequential and parallel composition of processes.

Exercise 7

With caps and cups one builds a notion of transposition:

$$\widehat{f} \;\mapsto\; \widehat{f} \;:=\; \widehat{f}$$

Verify that it coincides with transposition in the original theory, i.e.

$$\text{double}\left(f \right) = \widehat{f}$$

One may thus conclude that doubling preserves string diagrams. Thus, any of the calculations done for diagrams of linear maps lifts to pure quantum maps by doubling all of the diagrams. The converse is a bit more tricky: to go back to the theory of linear maps one needs to reintroduce global phases. Formally, for $\mathbf{D}, \mathbf{D}'$ arbitrary diagrams in the theory of pure quantum maps,

$$\left(\exists e^{i\alpha} : \quad D \quad = e^{i\alpha} \quad D' \quad \right) \;\Longleftrightarrow\; \widehat{D} \;=\; \widehat{D}'$$

To verify the right-to-left implication it suffices to show that for any linear maps f and g such that

$$\widehat{f} \;=\; \widehat{g}$$

there exists a α such that $\mathsf{f} = e^{i\alpha}\mathsf{g}$. Consider the following two scalars

$$\lambda \;:=\; f \; f \qquad\qquad \mu \;:=\; g \; f$$

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and observe that

$$\lambda\,\bar\lambda \;=\; \text{[diagram]} \;=\; \text{[diagram]} \;=\; \mu\,\bar\mu$$

Suppose $\lambda \neq 0$. Then one can divide both sides of the equation by $\lambda\bar\lambda$ yielding

$$1 \;=\; \frac{\mu\,\bar\mu}{\lambda\,\bar\lambda} \;=\; \frac{\mu}{\lambda}\,\overline{\left(\frac{\mu}{\lambda}\right)}$$

which means that $\frac{\mu}{\lambda}$ is a global phase, i.e. there is a α such that $\frac{\mu}{\lambda} = e^{i\alpha}$. Thus

$$\lambda\,\text{[diagram]} \;=\; \text{[diagram]} \;=\; \text{[diagram]} \;=\; \mu\,\text{[diagram]}$$

leading to $f = e^{i\alpha}g$. The other possibility corresponds to $\lambda = 0$, i.e.

$$\text{[diagram]} \;=\; \text{[diagram]} \;=\; \lambda \;=\; 0$$

By positive definiteness $f = 0$, thus $\hat{f} = 0$ and, by assumption, $\hat{g} = 0$. This can only be the case if $g = 0$, which may be concluded by attaching cups/caps to $\hat{g}$, i.e.

$$\text{[diagram]} \;=\; 0$$

and applying again positive definiteness. So, also in this case, $f = e^{i\alpha}g$ for any α.

It is important to notice that the proof is purely diagrammatic: scalars λ and μ are defined through diagrams and the proof proceeds by diagram substitution. The only place the structure of linear maps is used, namely the fact that scalars are complex numbers, is when formulating the result in terms of an expressing involving $e^{i\alpha}$ (which is also the reason to consider the two cases mentioned) — but see [1] for a complete general proof without assuming this strucutre for scalars. This means that doubling is in fact a procedure that can be applied to different process theories with the effect of getting rid of (a generalised notion of) global phases, therefore identifying processes that differ only by them.
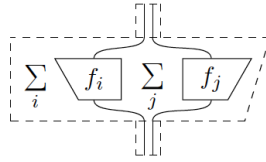
Prove that $\hat{f}$ is unitary iff f is.

Prove that $\hat{f}$ is a projector iff there exists a a projector g such that $\hat{f} = \hat{g}$.

Note, however, that sums in the doubled theory are not doubled sums. Actually, doubling a sum may even not lead to a pure quantum process. This is because doubling a sum involves two independent summations (i.e. over different indices):

$$\sum_i f_i \quad \sum_j f_j$$

which can be split into two sums for $i = j$ and $i \neq j$:

$$\sum_i f_i \, f_i \quad + \quad \sum_{i \neq j} f_i \, f_j$$
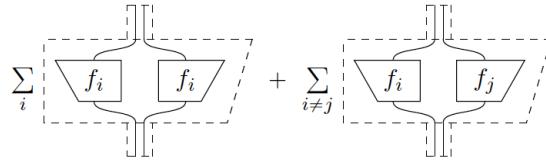
Thus,

$$\mathsf{double}\left(\sum_i f_i \right) = \sum_i \hat{f}_i \quad + \quad \sum_{i \neq j} f_i \, f_j$$

In general this extra term will not be 0. For example, for $\lambda_1 = \lambda_2 = 1$, one gets

$$\mathsf{double}\left(\sum_i \lambda_i \right) = \mathsf{double}(1 + 1) = 4 \neq 2 = 1 + 1 = \sum_i \lambda_i$$

This is a fundamental observation: sums in the theory of linear maps capture quantum *superpositions*. In the theory of pure quantum maps on the other hand, sums capture uncertainty about which process actually happened. They correspond to *mixed* quantum states.

Another element that is not preserved by doubling concerns orthonormal bases. Actually, doubling a basis with more than one state does not yield a basis in the theory of pure

quantum maps. A counterexample is provided by the following states over a basis $\mathcal{B}$.

$$\psi := \sum_j \boxed{j} \qquad \qquad \phi := \sum_j e^{i\alpha_j} \boxed{j}$$

where all parameters α_i are distinct. Since ϕ has at least two terms with non-equal coefficients $e^{i\alpha_j}$, the two states are not within a global phase of each other, which leads us to conclude that

$$\widehat{\psi} \neq \widehat{\phi}$$

However one can show that

$$\widehat{\psi} \quad = \quad \widehat{\phi}$$

which implies that doubling $\mathcal{B}$ does not yield a basis. It can be proved, however, that each basis for a type A in linear maps can be extended to a (non-orthogonal) basis in linear maps for the type $A \otimes A$, consisting entirely of pure quantum maps. So, in particular, this new basis is also a basis in the theory of pure quantum maps for the type $\hat{A}$.

References

[1] B. Coecke and A. Kissinger. *Picturing Quantum Processes: A First Course in Quantum Theory and Diagrammatic Reasoning.* Cambridge University Press, 2017.