

QUANTUM GROUP

Categorical Models of Quantum Circuits

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I. ABSTRACT

It is shown that equations that hold in appropriate monoidal categories have an explicit representation in terms of quantum circuits. Hence, we adjust and map the graphical calculus of Abramsky and Coecke’s categorical axiomatization of quantum theory onto quantum circuits, making a suitable extension applicable to problems stated in the language of quantum information science. Viewed in this new way, circuit diagrams themselves now become *arrows* in a Category, making quantum circuits a special case of a much more general mathematical framework. By building a precise connection between the quantum circuit language and the categorical model, we were able to use this new framework to produce results new to both areas. This should lead to more cross communication between the field of Categorical Quantum Theory, and Quantum Information Science.

II. INTRODUCTION

The theory of categories allows one to study the mathematical structures formed by the composition of quantum states. Consider the single-qubit operations: the identity operator, which is represented as a wire in a quantum circuit, and the NOT operation, represented as a \oplus on top of a wire (see¹ for background on quantum circuits). In quantum computation, the identity operator on a single qubit is given as a map: $\mathbf{1}_2 = |0\rangle\langle 0| + |1\rangle\langle 1|$, and NOT is given as $\sigma^x := |0\rangle\langle 1| + |1\rangle\langle 0|$. These are maps taking state vectors in the qubit Hilbert space \mathbb{C}^2 back to the qubit Hilbert space \mathbb{C}^2 . Viewed in another way, both σ^x and $\mathbf{1}$ are *arrows* with the same domain and codomain, that is arrows: $\mathbb{C}^2 \xrightarrow{\sigma^x} \mathbb{C}^2$ and $\mathbb{C}^2 \xrightarrow{\mathbf{1}} \mathbb{C}^2$.

Now let’s consider the states $\Phi^+ = |00\rangle + |11\rangle$ and $\Psi^+ = |01\rangle + |10\rangle$. In which ways are these states considered maps? It is claimed that in the most elementary case these states are maps from the complex numbers into the Hilbert space of two qubits $\mathbb{C}^2 \otimes \mathbb{C}^2$, that is they are arrows $\mathbb{C} \xrightarrow{\Phi^+} \mathbb{C}^2 \otimes \mathbb{C}^2$ and $\mathbb{C} \xrightarrow{\Psi^+} \mathbb{C}^2 \otimes \mathbb{C}^2$. To see this, simply pick a number $k \in \mathbb{C}$. Now Φ^+ acting on k is given as $\Phi^+(k) = k \cdot \Phi^+ \in \mathbb{C}^2 \otimes \mathbb{C}^2$, so Φ^+ took the arbitrary number k into the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$, and is thus an arrow $\mathbb{C} \xrightarrow{\Phi^+} \mathbb{C}^2 \otimes \mathbb{C}^2$ (by linearity $k = 1$ uniquely determines Φ^+).

There exists a canonical isomorphism (illustrated with the identity $\mathbf{1}$)

$$\begin{aligned} \mathbb{C}^2 \rightarrow \mathbb{C}^2 &\leftrightarrow \mathbb{C} \rightarrow \mathbb{C}^2 \otimes \mathbb{C}^2 \leftrightarrow \mathbb{C}^2 \otimes \mathbb{C}^2 \rightarrow \mathbb{C} \\ |0\rangle\langle 0| + |1\rangle\langle 1| &\leftrightarrow |00\rangle + |11\rangle \leftrightarrow \langle 00| + \langle 11| \end{aligned}$$

so every map from $\mathbb{C}^2 \rightarrow \mathbb{C}^2$ gives rise to exactly one map $\mathbb{C} \rightarrow \mathbb{C}^2 \otimes \mathbb{C}^2$ (see Theorem III.3), but we already saw that maps from \mathbb{C} into $\mathbb{C}^2 \otimes \mathbb{C}^2$ are themselves state vectors. (we could have equally well illustrated this isomorphism with $|000\rangle + |111\rangle \leftrightarrow |00\rangle\langle 0| + |11\rangle\langle 1|$, etc.). Every map of *type* $\mathbb{C}^2 \rightarrow \mathbb{C}^2$ gives rise to one state in $\mathbb{C}^2 \otimes \mathbb{C}^2$ and likewise, every map $\mathbb{C}^2 \rightarrow \mathbb{C}^2$ gives rise to exactly one costate, which is a map of type $\mathbb{C}^2 \otimes \mathbb{C}^2 \rightarrow \mathbb{C}$.

a. Structure This paper will continue by explaining how quantum circuits can be viewed as string diagrams. We will consider classical structures in the categorical quantum circuit model in Section IV. In Section V Oh we develop and present the graphical rewrite rule we call *gate-copy*. Before concluding we present an applications section which details how to construct quantum circuits to realise *W*-class states, and apply gate-copy to reduce a text book quantum simulation circuit.

III. STRING DIAGRAMS AS QUANTUM CIRCUITS

Category Theory provides the precise arena of mathematics concerned with diagrammatic reasoning. These diagrams capture mathematical properties of how maps, or arrows compose. Quantum circuits are only a subclass (planar and directed acyclic) of the types of *circuits* constructable in a Monoidal Category. For instance, By dropping temporal ordering during diagrammatic manipulation, we show how to reason about quantum circuits in new ways, and then translate the network back into a machine readable quantum circuit, to construct implementable

quantum processes, depending on specific application. Consider the following diagram (and then the following Theorem) showing the correspondence between the NOT gate, the singlet, and its costate:

$$\left(\oplus \right)^{|01\rangle + |10\rangle} \leftrightarrow \text{---} \oplus \text{---} \leftrightarrow \left(\oplus \right)^{|01\rangle + |10\rangle}$$

Theorem III.1. (*Bending quantum circuit wires*) *Bends in quantum circuit wires can correspond to dropping temporal ordering during diagrammatic manipulation. After diagrammatic manipulation the network can be translated back into a machine readable quantum circuit, to construct implementable quantum processes, depending on the specific application.*

The mathematical insight behind using pictures to represent tensor networks dates back to Penrose and in quantum circuits, notably to Deutsch. We make use of some of the mathematical ideas appearing in Abramsky and Coeckes Categorical Quantum Theory^{2,3}. The mathematics behind the category theory is based largely on a completeness result (originally proved by Joyal and Street) about the kinds of string diagrams we consider here.

Theorem III.2. Coherence for monoidal categories: *The geometric picture calculus in the plane faithfully represents calculations in monoidal categories.*

b. **States** We represent quantum states as follows:

$$\triangleleft \leftrightarrow |0\rangle + |1\rangle \quad \triangleleft \leftrightarrow |0\rangle$$

Other states are represented by changing the internal label inside the triangle, and costates (e.g. $\langle 0|$, $\langle +|$ etc.) are represented by reflecting across the vertical of the page (using the \dagger functor — see⁴), so the triangle instead points to the right.

c. **Wires** Defining identity as a composition of linear maps is done by considering the introduction of the linear operators to prove Theorem (III.3)

$$\eta := \sum_i |i\rangle \otimes |i\rangle \quad \text{and} \quad \epsilon := \sum_i \langle i| \otimes \langle i| \quad (1)$$

Theorem III.3. (Bracket-Duality) *There exists an isomorphism Ω for each state/map ψ sending $|\psi\rangle \longleftrightarrow \langle\psi|$.*

Proof. We first provide a map between a state/map $|\psi\rangle$ and its transpose. Using $\epsilon(\mathbf{1} \otimes |\psi\rangle) = \sum_i \langle i| \otimes \langle i|\psi\rangle = \sum_i \langle i|\psi\rangle \langle i| = \langle\psi|$ and $(\langle\psi| \otimes \mathbf{1})\eta = \sum_i \langle\psi|i\rangle \otimes |i\rangle = |\psi\rangle$. Now we consider the invertible (anti-linear) map, $\overline{(-)} : \mathbb{C} \rightarrow \mathbb{C}^* :: k \mapsto \bar{k}$ now using this map which defines complex conjugation together with the maps defined above gives Ω , (note that they commute) which establishes *bracket-duality*. \square

This so-called bra-ket duality, allows one to define the identity morphism by considering duality of the appropriate bra/ket of ϵ/η . (See Figure 1 for how this map can be used to take a transpose).

$$\text{S} \xleftrightarrow{\text{yanking}} \text{---} \quad \left(\text{---} \xleftrightarrow{\text{symmetry}} \text{---} \right)$$

d. **Compactness: Bell States as Cups and Caps** Our goal is to examine each component of a quantum circuit, and hence to examine the different two (e.g. maps and wires) and three-legged (e.g. dots) parts under map-state duality. We will soon justify that:

- (i): The copy operation given by a black dot (\bullet) in a quantum circuit with three connected wires can, under bra-ket duality be viewed as a multiplication taking elements from $\mathbb{C}^2 \rightarrow \mathbb{C}^2 \otimes \mathbb{C}^2$ or equivalently as a GHZ-state.
- (ii): The unit (identity) of the multiplication \bullet is given as $|+\rangle := |0\rangle + |1\rangle$ and for the multiplication \oplus as $|0\rangle$.
- (iii): Likewise from (ii), the dot (\oplus) meant to represent XOR addition, under map state duality, defines a multiplication as well a GHZ-state, but this time in the $|\pm\rangle$ basis, instead of the $|0/1\rangle$ basis for \bullet .

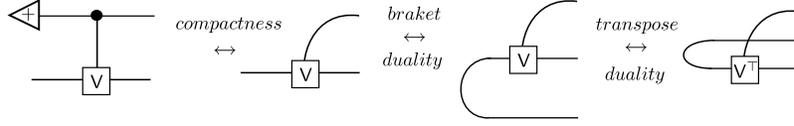


FIG. 1. A figure showing several rewrite rules applied to the controlled V-gate, starting with compactness of the black-dot and so the first two figures can be interchanged. The duality rewrite rule one from the rightmost (e.g. bending a wire) equivalent to preparing a Bell state and is justified by considering the action of the linear map $\epsilon := \sum_i \langle i | \otimes \langle i |$. The rightmost diagrams can be interchanged under transpose duality.

It is easy to verify in the circuit language that, under map state duality, the unit for the multiplication for \oplus generates the Bell-state $|00\rangle + |11\rangle$ when applied to \bullet and vice-versa (see Figure 2). Likewise, when considering the unit for \bullet under map-state duality, one generates the same Bell state. As noted by Coecke and Duncan in⁴, this is called a *compact structure* in category theory. Hence these multiplications, \bullet and \oplus , share the same compact structure, and so the categorical quantum circuit algebra has the graphical rewrites shown in Figure 2.

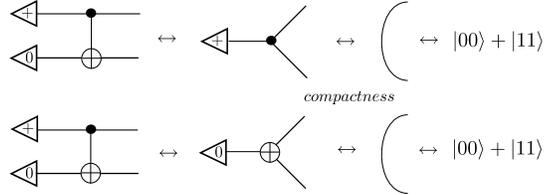
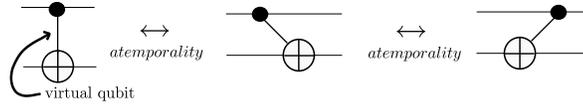
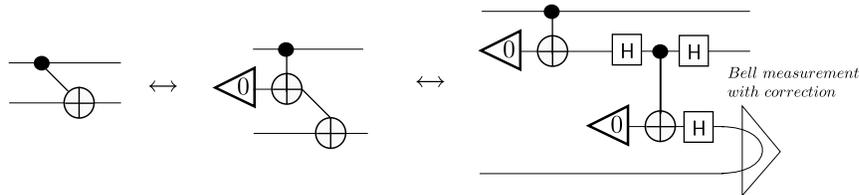


FIG. 2. Showing that the compact structure of the product \oplus is the same as the compact structure of the product \bullet . Here the compact structure of the black-dot is used in the lower picture to recover the plus-dot and vice versa. The compact structure of both dots produce the same cup as $\Phi^+ = |00\rangle + |11\rangle = |++\rangle + |--\rangle$ that is, Φ^+ is invariant under a Hadamard transform. The other three Bell-states can be generated by acting on one of the wires with a NOT-gate, a Z-gate and finally both.

e. Transforming Atemporal Graphs into Casually Connected Quantum Processes In circuit diagrams, the wires going up and down on the page are *logical connections*. These logical connections can be replaced with qubits, and we call such wires, *virtual qubits*. Consider the following figure and example.



Example III.4. *Atemporality can result in several equivalent physical realisations of the same network. Consider the following circuit which realises the middle circuit above.*



The circuit on the left must be transformed for realisation on a quantum processor. The equivalent circuit on the right is casually connected, provided all of the operations are preformed from left to right, including the Bell-basis measurement with correction. Caps at the ends (on the right) of a circuit appear to be diagrams that are directed backwards in time.

Remark III.5. *Typically in quantum circuits, at each time slice (that is vertically divided between gates), one will factor the network into a sequence of gates, each of which is unitary. In the general networks considered here, although each time-slice is a valid quantum process, each slice does not always represent a unitary map.*

f. Copy constructs: ‘Dots’ The quantum no-cloning theorem limits copying to any single basis. As $|0\rangle$ and $|1\rangle$ are eigenstates of σ^z , Z-copy is defined as Z-copy : $|00\rangle\langle 0| + |11\rangle\langle 1|$ and under bra-ket duality (on the right bra) this state becomes a GHZ-state as $\psi_{\text{GHZ}} = |000\rangle + |111\rangle$ and finally, the σ^z copy is given diagrammatically in Figure 3 (Top).

Figure 3 depicts X-copy (Bottom) — this spans the truth table for XOR as follows. If we consider $f(a, b) = a \oplus b$ then $f = 0$ corresponds to $(a, b) = (0, 0), (1, 1)$ and $f = 1$ corresponds to $(a, b) = (1, 0), (0, 1)$. Under bra-ket duality, the state defined by X-copy is given as $\sum_{ab} |a\rangle|b\rangle|f(a, b)\rangle = \psi_{\oplus} := |000\rangle + |110\rangle + |011\rangle + |101\rangle$ which is in the GHZ-class — as $\psi_{\oplus} = H \otimes H \otimes H(|000\rangle + |111\rangle)$. The X-copy operation is defined on a basis as

$$\text{X-copy} : \mathbb{C}^2 \rightarrow \mathbb{C}^2 \otimes \mathbb{C}^2 :: \begin{cases} |0\rangle \mapsto |00\rangle + |11\rangle \\ |1\rangle \mapsto |10\rangle + |01\rangle \end{cases} \quad \text{or equivalently} \quad \begin{cases} |+\rangle \mapsto |++\rangle \\ |-\rangle \mapsto |--\rangle \end{cases}$$

g. Dot-duality: Hadamard transforms between Z- and X-copy By dot-duality, the Z- and X-copy constructs are related by Hadamard transforms, applied to all of the dots legs to transform a Z- into an X-copy and vice versa — see Figure 3. This can be captured diagrammatically in the slightly different form (which clarifies several applications).

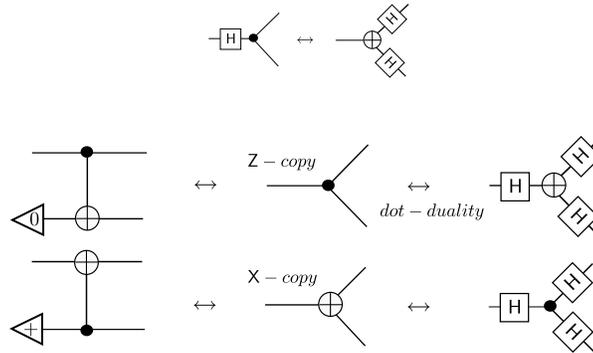


FIG. 3. Z- and X-copy constructs from the CNOT-gate.

IV. UNIVERSAL CLASSICAL STRUCTURES IN CATEGORICAL QUANTUM CIRCUITS

In classical computer science, a universal set of gates, is able to express any n -bit Boolean function $f : \mathbb{B}^n \rightarrow \mathbb{B} :: (x_1, \dots, x_n) \mapsto f(x_1, \dots, x_n)$. Universal sets include $\{\text{NAND}\}$, $\{\text{AND, OR, NOT}\}$, $\{\text{AND, XOR, 1}\}$ and others. One can also consider the states ψ formed by the bit patterns of these functions $f(a, b)$ as $\psi_f = \sum_{a,b \in \{0,1\}} |a\rangle|b\rangle|f(a, b)\rangle$.

In the following Table (IV) we illustrate the three qubit states representing the classical function of two-inputs. Explicitly, one can realise all the states on the right side of the table using the circuit presented in Figure 5 (Right — see the caption). This circuit allows one to realize all quantum states with a bit pattern given by the truth table of some defined Boolean function. Also applicable to many quantum information processing tasks, consider the subset of qubit quantum mechanics consisting of equally weighted arbitrary superposition of quantum states, where each term can have a relative phase of $+1$ or -1 . To realise states in this class one can combine both circuits presented in Figure 5.

Remark IV.1. (*Boolean States*) Any quantum state with equal amplitudes which has a bit pattern related to that of a Boolean function $\psi_f = \sum_{\bar{x} \in \{0,1\}^n} |\bar{x}\rangle|f(\bar{x})\rangle$ can be realised by post selection and composition of the states given in Figure 5. In addition, local phase terms can be added using the controlled gate in Figure 5, allowing the realisation of states $\psi_f = \sum_{\bar{x} \in \{0,1\}^n} a_{\bar{x}} |\bar{x}\rangle|f(\bar{x})\rangle$.

non-linear	linear (Frobenius Algebras — see V 0 h)
$\psi_{\text{AND}} = 000\rangle + 010\rangle + 100\rangle + 111\rangle$	$\psi_{\text{XOR}} = 000\rangle + 011\rangle + 101\rangle + 110\rangle$
$\psi_{\text{OR}} = 001\rangle + 011\rangle + 101\rangle + 111\rangle$	$\psi_{\text{XNOR}} = 001\rangle + 010\rangle + 100\rangle + 111\rangle$
$\psi_{\text{NAND}} = 001\rangle + 011\rangle + 101\rangle + 110\rangle$	
$\psi_{\text{NOR}} = 001\rangle + 010\rangle + 100\rangle + 110\rangle$	

FIG. 4. The bit pattern of these quantum states represents a Boolean function (given by the subscript) such that the right most bit is the Boolean functions output, and the two left bits are the functions inputs, and the non-linear Boolean functions are on the left side of the table and the linear functions on the right. Consider the state ψ_{AND} , and Boolean variables x_1 and x_2 , then the superposition ψ_{AND} encodes the function $|x_1, x_2, x_1 \wedge x_2\rangle$ in each term in the superposition, and $\psi_{\text{AND}} = \sum_{x_1, x_2 \in \{0,1\}} |x_1, x_2, x_1 \wedge x_2\rangle$. As outlined in the text, map state-duality allows us (for instance) to express this state as the operator $|0\rangle\langle 00| + |0\rangle\langle 01| + |0\rangle\langle 10| + |1\rangle\langle 11| :: |x_1, x_2\rangle \mapsto |x_1 \wedge x_2\rangle$ which projects qubit states to the AND of their bit value.

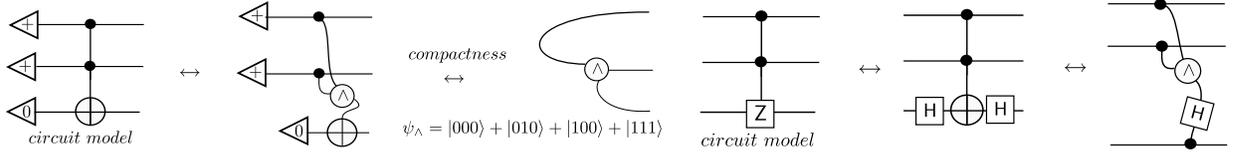


FIG. 5. (Left) Illustrates the use of compact structures for black and plus dots to prepare the state $\psi_{\text{AND}} = |000\rangle + |010\rangle + |100\rangle + |111\rangle$ (where the symmetry of the upper two wires was used). Using only single qubit NOT-gates, one can use this method to construct any of the states representing the non-linear functions in Figure IV. (Right) Considering the example shown in Figure 5, one can construct a double controlled σ^z -gate using the dot-duality rewrite rule from Section III 0 g. As with the right circuit, this circuit on the left can similarly be used to create the state $|00+\rangle + |01+\rangle + |10+\rangle + |11-\rangle$.

V. GHZ- AND W-PRODUCTS

In the Categorical Model of Quantum Circuits, every quantum state of three or more systems forms a *product*. By this it means that the measurement outcomes have a mathematical structure which can be viewed as a type of multiplication. For instance, if one measures the first bit of a GHZ-state in the σ^x -basis and recovers $+1$, the state of the system is left in a Bell state, which under bra-ket duality is an identity wire as the state $|+\rangle$ is a unit for the multiplication. Let's begin with the following depiction of the state induced GHZ- and W-products (the W-state is defined in Section VI 0 j).

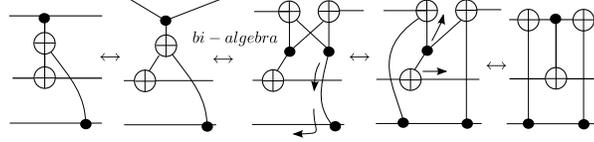
$$\begin{array}{ccc}
 \begin{array}{c} a|0\rangle + b|1\rangle \\ \\ c|0\rangle + d|1\rangle \end{array} & \begin{array}{c} \diagdown \\ \bullet \\ \diagup \end{array} & a \cdot c|0\rangle + b \cdot d|1\rangle \\
 & & \\
 \begin{array}{c} a|0\rangle + b|1\rangle \\ \\ c|0\rangle + d|1\rangle \end{array} & \begin{array}{c} \diagdown \\ \circ \\ \diagup \end{array} & a \cdot c|0\rangle + (a \cdot d + b \cdot c)|1\rangle
 \end{array}$$

Here one typically considers the numbers a, b, c, d to be amplitudes of a quantum state after measurement, e.g. measuring a state in σ^y and recovering a -1 would result in $|y_-\rangle$, that is $(a, b) = (1, -i)$, etc. This will be made precise below.

The GHZ state has the nice property that it is symmetric under particle exchange — meaning the induced product is associative. By composition of the GHZ-state with cap operators, one constructs the operator $|00\rangle\langle 0| + |11\rangle\langle 1| : \mathbb{C}^2 \rightarrow \mathbb{C}^2 \otimes \mathbb{C}^2 :: |i\rangle \mapsto |i, i\rangle$ which we already know acts as a copy operation on the basis $|0\rangle, |1\rangle$, for $i \in \{0, 1\}$.

Consider again the map given by $|0\rangle\langle 00| + |1\rangle\langle 11| : \mathbb{C}^2 \rightarrow \mathbb{C} :: (a|0\rangle + b|1\rangle) \otimes (c|0\rangle + d|1\rangle) \mapsto ac|0\rangle + bd|1\rangle$ which is readily verified by considering the action of the map on states with amplitude coefficients (a, b) and (c, d) . Hence, the GHZ product forms a monoid (M, \cdot, e) as follows: M is the space \mathbb{C}^2 , and e is given by the $|+\rangle$ now the product becomes $\text{GHZ} : \mathbb{C}^2 \otimes \mathbb{C}^2 \mapsto \mathbb{C}^2 :: (a, b) \cdot (c, d) \mapsto (ac, bd)$ with unit $(1, 1)$. Again we note that these amplitudes are measurement outcomes, and so one can think of post-selection as being built into the induced product structure.

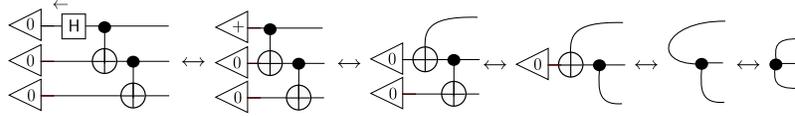
Definition V.1. (GHZ-product) *The GHZ-product with respect to the state $|000\rangle + |111\rangle$ is given as $\text{GHZ} : \mathbb{C}^2 \otimes \mathbb{C}^2 \mapsto \mathbb{C}^2 :: (a, b) \cdot_G (c, d) \mapsto (ac, bd)$ where $(a, b), (c, d)$ represent the complex amplitudes of the state after measurement. The unit of the multiplication is $|+\rangle := (1, 1)$.*



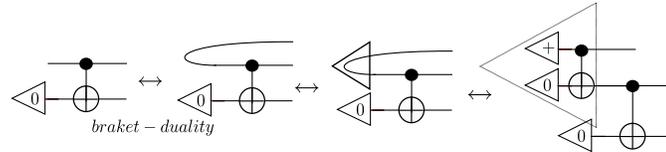
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VI. APPLICATIONS

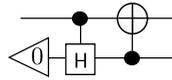
i. GHZ-class circuits In the present manuscript we considered dualised forms of the GHZ-state. This state can be realised by the following circuit:



The simplification from left to right first uses the self-duality of the H-gate, and then the compact structures of the dots. On the other hand, one could realise this circuit by considering bra-ket-duality of the copy operation found from letting a CN-gate act on $|0\rangle$. Diagrammatically this provides backwards justification of the circuit realisation as follows. These circuits scale to create n -qubit GHZ-states in the evident way.

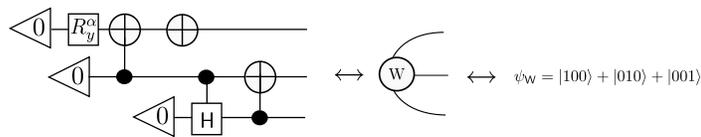


j. W-class circuits We will now use bra-ket duality to develop a circuit to realise W-states — these are outside the stabiliser class as $-\sigma^z\sigma^z\sigma^z$ is W's only Pauli stabiliser. First consider $|001\rangle + |010\rangle + |100\rangle = \sigma_1^x(|101\rangle + |110\rangle + |000\rangle)$ and so $\psi_W = |101\rangle + |110\rangle + |000\rangle$ becomes our representative of the W-class. As described, the W-product forms a map so the first step is to find a unitary U and a fixed state ψ such that $U|0\rangle \otimes |\psi\rangle = |0\rangle \otimes |0\rangle$ and $U|0\rangle \otimes |\psi\rangle = |01\rangle + |10\rangle$ we let $\psi := |0\rangle$ and with a little trial and error we arrive at



One will then naturally attempt to dualise the circuit by bending the top wire. This however fails as follows. The input state to the circuit is now $(|00\rangle + |11\rangle)|0\rangle$ the controlled H-gate takes this to $|000\rangle + \frac{1}{\sqrt{2}}(|111\rangle + |110\rangle)$ and then the CN-gate takes this to $|000\rangle + \frac{1}{\sqrt{2}}(|101\rangle + |110\rangle)$.

Normalisation can now be accounted for by constructing a generalised cup, which realises the following state: $\cos(\alpha)|00\rangle + \sin(\alpha)|11\rangle$ for $\cos(\theta) = \sqrt{2/3}$. This can be realized by the following sequence $(R_y(\alpha) \otimes \mathbf{1})(\text{CNOT})|00\rangle = \cos(\alpha)|00\rangle + \sin(\alpha)|11\rangle$, for $R_y(\alpha) = \exp[-i\alpha\sigma^y]$ and the full circuit becomes



k. Circuit simplification using Gate-copy In Figure 6, we apply gate-copy to simplify a circuit designed to simulate time evolution under the $\sigma^z\sigma^z\sigma^z$ Hamiltonian.

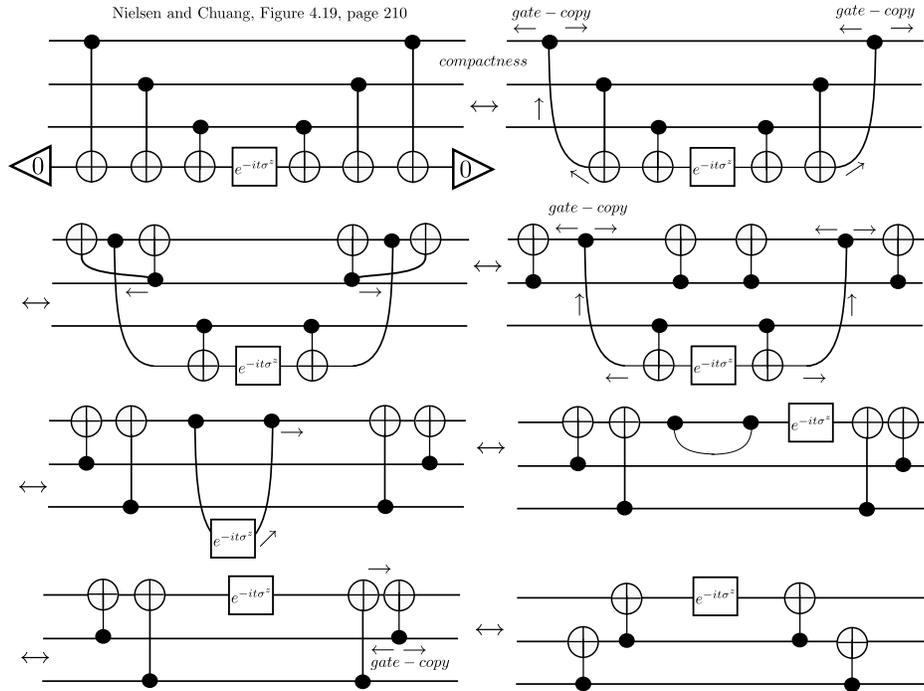


FIG. 6. Starting from the circuit from Figure 4.19 on page 210 of⁶, we apply the compact structure and then use the Gate-copy reduction rule introduced in Theorem V.8 to simply this network to it's form on the bottom right.

VII. CONCLUSION

We used a categorical quantum circuit model to provide explicit constructions for non-stabiliser quantum states generating universal *real*-qubit quantum theory. We then applied this new model to develop quantum circuits generating states in the *W*-class. Finally, graphical rewrites were developed to reduce a text book quantum simulation circuit.

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