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Quantum Circuit Completeness: Extensions and Simplifications

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Abstract

Although quantum circuits have been ubiquitous for decades in quantum computing, the first complete equational theory for quantum circuits has only recently been introduced. Completeness guarantees that any true equation on quantum circuits can be derived from the equational theory.

We improve this completeness result in two ways: (i) We simplify the equational theory by proving that several rules can be derived from the remaining ones. In particular, two out of the three most intricate rules are removed, the third one being slightly simplified. (ii) The complete equational theory can be extended to quantum circuits with ancillae or qubit discarding, to represent respectively quantum computations using an additional workspace, and hybrid quantum computations. We show that the remaining intricate rule can be greatly simplified in these more expressive settings, leading to equational theories where all equations act on a bounded number of qubits.

The development of simple and complete equational theories for expressive quantum circuit models opens new avenues for reasoning about quantum circuits. It provides strong formal foundations for various compiling tasks such as circuit optimisation, hardware constraint satisfaction and verification.

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Keywords and phrases Quantum Circuits, Completeness, Graphical Language

1 Introduction

Introduced in the 80's by Deutsch [18], the quantum circuit¹ model is ubiquitous in quantum computing. Various quantum computing tasks – circuit optimisation, fault tolerant quantum computing, hardware constraint satisfaction, and verification – involve quantum circuit transformations [23, 33, 34, 35, 38]. It is therefore convenient to equip the quantum circuit formalism with an *equational theory* providing a way to transform a quantum circuit while preserving the represented unitary map. When the equational theory is powerful enough to guarantee that any true property can be derived, it is said to be *complete*, in other words, any two circuits representing the same unitary map can be transformed into one another using the rules of the equational theory.

The first complete equational theory (denoted QC_{old} in the following) for quantum circuits has been introduced recently [12]. This equational theory has been derived from the LOv-calculus [11], a language for optical quantum computing. Before that, complete equational theories were only known for non-universal fragments of quantum circuits, such as

¹ Originally called *Quantum Computational Networks*, the term *quantum circuits* is nowadays unanimously used.

Clifford+T circuits acting on two qubits [6, 15], Clifford+CS circuits acting on three qubits [7], the stabiliser fragment [32, 42], the CNot-dihedral fragment [1], or fragments of reversible circuits [24, 14, 13].

The quantum circuit model can naturally be extended to encompass ancillary qubits, measurements, or qubit discarding, in order to express more general evolutions like isometries and completely positive trace preserving maps. In a model of quantum circuits with ancillae, one can use an additional work space by adding fresh qubits, as well as releasing qubits when they are in a specific state. Even if the vanilla quantum circuits form a universal model of quantum computation,² this additional space is useful in many cases. It is for instance commonly used for the construction of quantum oracles.³ Another important example is the parallelisation of quantum circuits: ancillae enable a better parallelisation of quantum gates, leading generally to a tradeoff between space (number of ancillae) and depth (parallel time) [36]. Notice that ancillae should be carefully used as the computation should leave a clean work space: one can only get rid of a qubit at the end of the computation if this qubit is in the $|0\rangle$ -state.

We also consider another extension of quantum circuits where arbitrary qubits can be discarded (or traced out), whatever their states are. This extension allows for the representation of: (i) quantum measurements and more generally classically controlled computations; and (ii) arbitrary general quantum computations (CPTP maps⁴). Such quantum circuits can be used to deal with fault-tolerant quantum computing and error correcting codes which, by construction, require an additional workspace, measurements and corrections. One can also represent measurement-based quantum computation [43, 16] with this class of circuits. The study of hybrid quantum-classical models is also a subject of interest in algorithmic and complexity theory [21, 2].

Contributions. We address here the problem of simplifying the complete equational theory QC_{old} . Obtained through a non-trivial translation from the LOv-calculus, QC_{old} involves non-trivial equations (see Figure 3), in particular Equation $(\text{K}_{\text{old}}^*)$ depicts a family of equations acting on an unbounded number of qubits, witness of the non-functoriality of the back and forth translations between quantum circuits and optical circuits, due to the fundamentally different interpretations of the parallel composition in the two circuit languages.

We show that several rules, including two of the three most intricate ones (Equations (12) and (13)), can actually be derived from the other rules, the third one (Equation $(\text{K}_{\text{old}}^*)$) being slightly simplified. This leads to a simpler, more compact and easier to use complete equational theory, which however still involves a family of equations acting on an unbounded number of qubits.

We consider the more expressive frameworks of quantum circuits with ancilla and/or discards. Several constructions for discarding [22, 9], measurements and quantum operations [45], allow one to turn the complete equational theory for vanilla quantum circuits into complete equational theories for quantum circuits with ancilla and/or discards, by adding a few extra equations. We then mainly show that in these more expressive setting, the unbounded family of equations $(\text{K}_{\text{old}}^*)$ can be derived from bounded ones, leading to complete equational theories acting on a most three qubits.

² Any n -qubit unitary transformation can be implemented by a n -qubit vanilla quantum circuit.

³ Implementation of the n -qubit unitary transformation $U_f : |x, y\rangle \mapsto |x, y \oplus f(x)\rangle$ given a classical circuit implementing the boolean function f [39].

⁴ Completely positive trace-preserving maps.

Related work. The first complete equational theory for a universal quantum computing model has been introduced in 2017 for the ZX-calculus [25]. Since then, complete equational theories have been introduced for other universal fragments of the ZX-calculus [26, 20, 27, 49, 28] and its variants ZH-, ZW-calculi [3, 19]. ZX-like languages differ from quantum circuits mainly in two ways: they are more expressive, allowing the representation of any matrix⁵ so in particular those representing post-selected evolutions for instance; the second major difference – and the most important in our context – is that not all the generators are unitary, thus even if a ZX-diagram represents an overall unitary evolution, it does not provide in general a (deterministic) implementation by means of elementary gates contrary to the quantum circuit model. To circumvent this problem one can consider the so-called subclass of circuit-like ZX-diagrams which is in one-to-one correspondence with quantum circuits, however this class is not closed under the known complete equational theories of the ZX-calculus. In particular, the problem of transforming a ZX-diagram representing a unitary evolution into a circuit-like one has been studied in the context of circuit optimisation [29], leading to various heuristics [30, 4, 17]. However, this approach fails so far to lead to a complete equational theory for quantum circuits.

The paper is structured as follows. In Section 2, we consider vanilla quantum circuits together with a new equational theory QC. We prove the completeness of QC first for the fragment of 1-CNot circuits,⁶ that we then use to derive the remaining equations of the already known complete equational theory QC_{old} introduced in [12]. In Section 3, we introduce an extension of vanilla quantum circuits with $|0\rangle$ -state initialisation. Universal for isometries, such quantum circuits with initialisation are introduced as an intermediate step towards circuits with ancillae and/or discard. We add to the equational theory QC two basic equations involving qubit-initialisation, and provide a proof of completeness of the augmented equational theory QC_{iso} using a particular circuit decomposition based on the so-called cosine-sine decomposition of unitary maps. The completeness of QC_{iso} is extended to provide complete equational theories for quantum circuits with ancillae (QC_{ancilla} in Section 4) – which additionally allow for the release of qubits when they are in a specific state – and for quantum circuits with qubit discarding (QC_{discard} in Section 5) – which allows the tracing out of any qubits. Both extensions provide alternative representations of multi-controlled gates, allowing the simplification of the remaining intricate rule – which acts on an unbounded number of qubits – into its 2-qubit version.


2 Vanilla quantum circuits

2.1 Graphical languages

We define quantum circuits using the formalism of props [31], which are, in category-theoretic terms, strict symmetric monoidal categories whose objects are generated by a single object, or equivalently with $(\mathbb{N}, +)$ as a monoid of objects. The prop formalism provides a formal and rigorous framework to describe graphical languages. The main features of props are recalled in the following. Circuits $C_1 : m \rightarrow n$ and $C_2 : p \rightarrow q$ in a prop, depicted as $m \begin{array}{|c|} \hline C_1 \\ \hline \end{array} n$ and $p \begin{array}{|c|} \hline C_2 \\ \hline \end{array} q$ can be composed: (1) “in sequence” $C_2 \circ C_1 : m \rightarrow q$ if $n = p$, graphically $m \begin{array}{|c|} \hline C_1 \\ \hline \end{array} \begin{array}{|c|} \hline C_2 \\ \hline \end{array} q$;

⁵ the only constraint is on the dimension of the matrices which must be a power of two for the qubit case, qudit versions also exist [8, 41]

⁶ The sub-class of quantum circuits made of at most one CNot gate.

(2) “in parallel” $C_1 \otimes C_2 : m + p \rightarrow n + q$, graphically . The *unit* for tensor product \otimes is the *empty circuit*: $\square : 0 \rightarrow 0$. This means $\square \otimes C = C = C \otimes \square$ for any circuit C . The circuit $\text{---} : 1 \rightarrow 1$ depicts the identity, $\text{---} \text{---} : 2 \rightarrow 2$ is the identity on two wires and more generally $\text{---}^{\otimes m} := \text{---} \otimes \text{---}^{\otimes m-1} : m \rightarrow m$ (with $\text{---}^{\otimes 0} := \square$) is the identity on m wires. Graphically, we obviously have $\text{---}^{\otimes n} \circ C = C = C \circ \text{---}^{\otimes m}$ for any $C : m \rightarrow n$. Finally, a prop is also endowed with a particular circuit $\text{---} \times \text{---} : 2 \rightarrow 2$ which satisfies $\text{---} \times \text{---} = \text{---}$. Graphically (and semantically in what follows) $\text{---} \times \text{---}$ swaps places. By compositions, we may build the following family of circuits

$$\begin{array}{c} \text{---} \\ \text{---} \end{array} \times \begin{array}{c} \text{---} \\ \text{---} \end{array} : m + n \rightarrow n + m$$

which exchanges m -sized and n -sized registers. In a prop, circuits satisfy a set of identities, that graphically translate as “being able to deform the circuit”. For instance, the following identities are valid transformations:

$$\begin{array}{c} \text{---} \\ \text{---} \end{array} \otimes \begin{array}{c} \text{---} \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \text{---} \end{array} \otimes \begin{array}{c} \text{---} \\ \text{---} \end{array} \quad \begin{array}{c} \text{---} \\ \text{---} \end{array} \times \begin{array}{c} \text{---} \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \text{---} \end{array} \times \begin{array}{c} \text{---} \\ \text{---} \end{array}$$

In the following, all the considered theories will be props, and hence will have the empty, identity and swap circuits as basic generators.

2.2 Vanilla quantum circuits and their equational theory

We first consider the vanilla model of quantum circuits generated by the very standard gateset: Hadamard, Phase gates, and CNot, together with global phases:

► **Definition 1.** Let **QC** be the prop generated by $\text{---} \text{---} : 1 \rightarrow 1$, $\text{---} \text{---} : 1 \rightarrow 1$, $\text{---} \oplus \text{---} : 2 \rightarrow 2$ and $\text{---} : 0 \rightarrow 0$ for any $\varphi \in \mathbb{R}$.

We associate with any quantum circuit its standard interpretation as a unitary map:

► **Definition 2 (Semantics).** For any n -qubit **QC**-circuit C , let $\llbracket C \rrbracket : \mathbb{C}^{\{0,1\}^n} \rightarrow \mathbb{C}^{\{0,1\}^n}$ be the semantics of C inductively defined as the linear map satisfying $\llbracket C_2 \circ C_1 \rrbracket = \llbracket C_2 \rrbracket \circ \llbracket C_1 \rrbracket$; $\llbracket C_1 \otimes C_2 \rrbracket = \llbracket C_1 \rrbracket \otimes \llbracket C_2 \rrbracket$; and






$$\llbracket \text{---} \rrbracket = 1 \mapsto 1 \quad \llbracket \text{---} \rrbracket = 1 \mapsto e^{i\varphi} \quad \llbracket \text{---} \text{---} \rrbracket = |x\rangle \mapsto \frac{|0\rangle + (-1)^x |1\rangle}{\sqrt{2}} \quad \llbracket \text{---} \text{---} \rrbracket = |x\rangle \mapsto e^{ix\varphi} |x\rangle$$

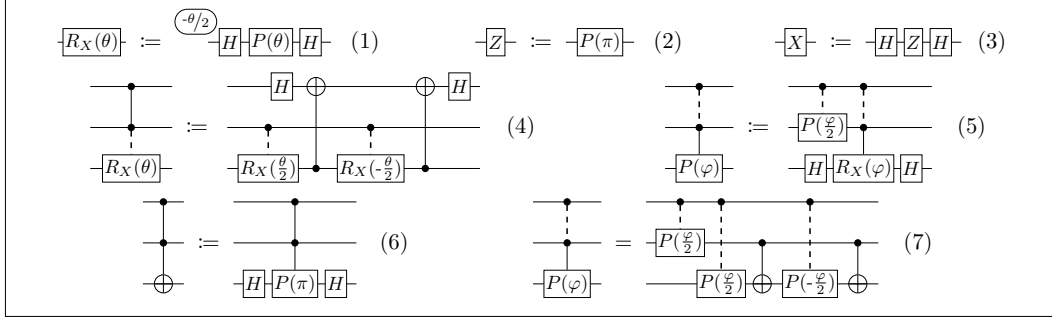
$$\llbracket \text{---} \oplus \text{---} \rrbracket = |x, y\rangle \mapsto |x, x \oplus y\rangle \quad \llbracket \text{---} \rrbracket = |x\rangle \mapsto |x\rangle \quad \llbracket \text{---} \times \text{---} \rrbracket = |x, y\rangle \mapsto |y, x\rangle$$

Note that for any **QC**-circuit C , $\llbracket C \rrbracket$ is unitary. Conversely, it is well known that any unitary map acting on a finite number of qubits can be represented by a **QC**-circuit:

► **Proposition 3 (Universality).** **QC** is universal, i.e. for any unitary $U : \mathbb{C}^{\{0,1\}^n} \rightarrow \mathbb{C}^{\{0,1\}^n}$ there exists a **QC**-circuit C such that $\llbracket C \rrbracket = U$.

Quantum circuits, as defined above, only have four different kinds of generators, however, it is often convenient to use other gates that can be defined by combining them. For instance, following [5, 12], Pauli gates, Toffoli, X -rotations, and multi-controlled gates are defined in Figure 1. Note that while the phase gate $\text{---} \text{---}$ is 2π -periodic, the X -rotation $\text{---} \text{---}$ is 4π -periodic.

We use the standard bullet-based notation for multi-controlled gates. For instance  denotes the application of a phase gate $\boxed{P(\varphi)}$ on the third qubit controlled by the first two qubits. With a slight abuse of notations, we use dashed lines for arbitrary number of control qubits, e.g.  : $n + 1 \rightarrow n + 1$ or simply  : $n + 1 \rightarrow n + 1$ have $n \geq 0$ control qubits (possibly zero), whereas  : $n + 2 \rightarrow n + 2$ and  : $1 + n + 1 \rightarrow 1 + n + 1$ have at least one control qubit.



■ **Figure 1** Shortcut notations for usual gates defined for any $\varphi, \theta \in \mathbb{R}$. Equation (1) defines X -rotations while Equations (2) and (3) define Pauli gates. Equations (4) and (5) are inductive definitions of multi-controlled gates. Equation (6) is the definition of the well known Toffoli gate. Equation (7) is an alternative definition of the multi-controlled phase gate that is proved to be equivalent to Equation (5) in Appendix B.3.

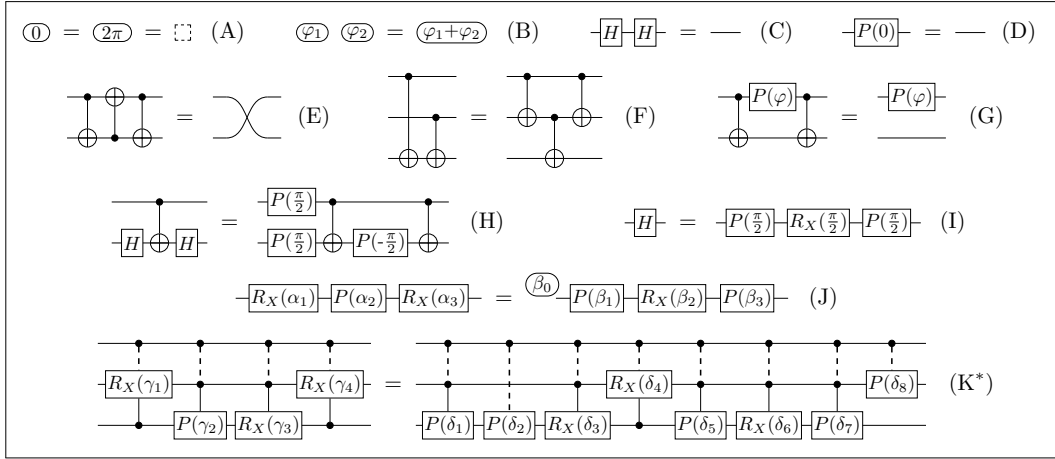
We equip the vanilla quantum circuits with the equational theory QC defined in Figure 2. We write $\text{QC} \vdash C_1 = C_2$ when C_1 can be transformed into C_2 using the equations of QC . More formally, $\text{QC} \vdash \cdot = \cdot$ is the smallest congruence which satisfies the equations of Figure 2 together with the deformation rules that come with the prop formalism. QC is sound, i.e. for any QC -circuits C_1, C_2 if $\text{QC} \vdash C_1 = C_2$ then $\llbracket C_1 \rrbracket = \llbracket C_2 \rrbracket$. This can be proved by observing that all equations of QC are sound.

Figure 3 depicts the complete equational theory QC_{old} for vanilla quantum circuits introduced in [12]. Compared to QC_{old} , Equations (8) and (9) are now subsumed by Equation (G) in QC , Equation (K^*) is a slight simplification of Equation (K_{old}^*) with one less parameter in the RHS circuit, whereas Equations (10) and (11) together with Equations (12) and (13) have been removed, as we prove in the following that they can be derived in QC .

2.3 Reasoning on quantum circuits

To derive an equation $C_1 = C_2$ over quantum circuits, one can apply some rules of the equational theory to transform step by step C_1 into C_2 . In the context of vanilla quantum circuits, we can take advantage of the reversibility of generators to *simplify* equations. Indeed, intuitively, proving $C_1 \circ \boxed{H} = C_2 \circ \boxed{H}$ is equivalent to proving $C_1 = C_2$ as \boxed{H} is (provably) reversible. Similarly, proving $C_1 = C_2$ should be equivalent to proving $C_1 \circ C_2^\dagger = \text{---}$, where the adjoint of a circuit is defined as follows:

► **Definition 4.** For any QC -circuit C , let C^\dagger be the adjoint of C inductively defined as $(C_2 \circ C_1)^\dagger := C_1^\dagger \circ C_2^\dagger$; $(C_1 \otimes C_2)^\dagger := C_1^\dagger \otimes C_2^\dagger$; and for any $\varphi \in \mathbb{R}$, $(\textcircled{\varphi})^\dagger := \textcircled{\varphi}$,



■ **Figure 2** Equational theory QC. Equations (B) and (G) are defined for any $\varphi, \varphi_1, \varphi_2 \in \mathbb{R}$. In Equations (J) and (K*) the LHS circuit has arbitrary parameters which uniquely determine the parameters of the RHS circuit. Equation (J) follows from the well-known Euler-decomposition which states that any unitary can be decomposed, up to a global phase, into basic X - and Z -rotations. Thus for any $\alpha_i \in \mathbb{R}$, there exist $\beta_j \in \mathbb{R}$ such that Equation (J) is sound. We make the angles β_j unique by assuming that $\beta_1 \in [0, \pi)$, $\beta_0, \beta_2, \beta_3 \in [0, 2\pi)$ and if $\beta_2 \in \{0, \pi\}$ then $\beta_1 = 0$. Equation (K*) reads as follows: the equation is defined for any $n \geq 2$ input qubits, in such a way that all gates are controlled by the first $n - 2$ qubits. Similarly to Equation (J), for any $\gamma_i \in \mathbb{R}$, there exist $\delta_j \in \mathbb{R}$ such that Equation (K*) is sound. We ensure that the angles δ_j are uniquely determined by assuming that $\delta_1, \delta_2, \delta_5 \in [0, \pi)$, $\delta_3, \delta_6, \delta_7, \delta_8 \in [0, 2\pi)$, $\delta_4 \in [0, 4\pi)$, if $\delta_3 = 0$ and $\delta_6 \neq 0$ then $\delta_2 = 0$, if $\delta_3 = \pi$ then $\delta_1 = 0$, if $\delta_4 \in \{0, 2\pi\}$ then $\delta_1 = \delta_3 = 0$, if $\delta_4 \in \{\pi, 3\pi\}$ then $\delta_2 = 0$, if $\delta_4 \in \{\pi, 3\pi\}$ and $\delta_3 = 0$ then $\delta_1 = 0$, and if $\delta_6 \in \{0, \pi\}$ then $\delta_5 = 0$.

$(-\overline{P(\varphi)})^\dagger := \overline{P(-\varphi)}$, and $g^\dagger := g$ for any other generator g .

► **Proposition 5.** $\llbracket C^\dagger \rrbracket = \llbracket C \rrbracket^\dagger$ for any QC-circuit C , where $\llbracket C \rrbracket^\dagger$ is the usual linear algebra adjoint of $\llbracket C \rrbracket$.

Proof. By induction on C . ◀

► **Proposition 6** (Simplification principle). For any n -qubit QC-circuits C, C_1, C_2

$$\text{QC} \vdash C \circ C_1 = C_2 \quad \Leftrightarrow \quad \text{QC} \vdash C_1 = C^\dagger \circ C_2$$

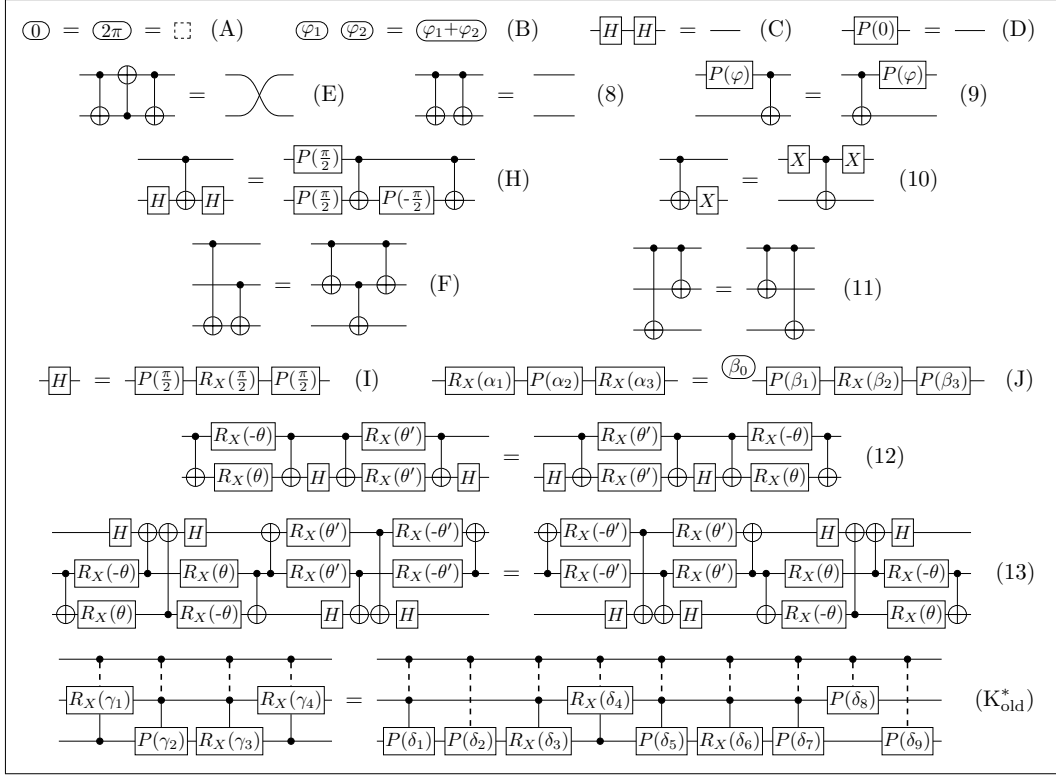
and

$$\text{QC} \vdash C_1 \circ C = C_2 \quad \Leftrightarrow \quad \text{QC} \vdash C_1 = C_2 \circ C^\dagger$$

Proof. First we show by induction that $\text{QC} \vdash C \circ C^\dagger = \text{---}^{\otimes n}$ and $\text{QC} \vdash C^\dagger \circ C = \text{---}^{\otimes n}$ for any C . Then, w.l.o.g. we show that $(\text{QC} \vdash C \circ C_1 = C_2) \Rightarrow (\text{QC} \vdash C_1 = C^\dagger \circ C_2)$: assuming $\text{QC} \vdash C \circ C_1 = C_2$, we have $\text{QC} \vdash C_1 = C^\dagger \circ C \circ C_1 = C^\dagger \circ C_2$. ◀

2.4 Completeness

We prove the completeness of QC by showing that every equation of the original complete equational theory QC_{old} introduced in [12] can be derived in QC. To this end we first show the completeness of QC for the (modest) fragment of quantum circuits containing at most one CNot gate.



■ **Figure 3** Equational theory QC_{old} introduced in [12]. Equations (A),(B),(C),(D),(E),(H),(F),(I) are (J) are also in the equational theory QC . Equation (K_{old}^*) is the old version of Equation (K^*) with one more parameter, and where the uniqueness of the parameters δ_j is given by the conditions: $\delta_1, \delta_2, \delta_5 \in [0, \pi)$, $\delta_3, \delta_4, \delta_6, \delta_7, \delta_8, \delta_9 \in [0, 2\pi)$, if $\delta_3 = 0$ then $\delta_2 = 0$, if $\delta_3 = \pi$ then $\delta_1 = 0$, if $\delta_4 = 0$ then $\delta_1 = \delta_3 (= \delta_2) = 0$, if $\delta_4 = \pi$ then $\delta_2 = 0$, if $\delta_4 = \pi$ and $\delta_3 = 0$ then $\delta_1 = 0$, and if $\delta_6 \in \{0, \pi\}$ then $\delta_5 = 0$. Note that these conditions on the δ_j for $1 \leq j \leq 8$ are the same as in Equation (K^*) except for δ_4 , which is restricted to be in $[0, 2\pi)$ instead of $[0, 4\pi)$, and for δ_2 , which has to be 0 when $\delta_3 = 0$ even if $\delta_6 = 0$.

► **Lemma 7** (1-CNot completeness). QC is complete for circuits containing at most one CNot , i.e. for any QC -circuits C_1, C_2 with at most one CNot , if $\llbracket C_1 \rrbracket = \llbracket C_2 \rrbracket$ then $\text{QC} \vdash C_1 = C_2$.

Proof. First we can show that, for semantic reasons, it is enough to prove the statement for 2-qubit circuits containing no swap gate and exactly one CNot gate. Then, by the simplification principle (Proposition 6), it is sufficient to prove

$$\begin{array}{c} \boxed{A} \\ \oplus \\ \boxed{B} \end{array} \begin{array}{c} \boxed{C} \\ \oplus \\ \boxed{D} \end{array} = \begin{array}{c} \oplus \\ \oplus \end{array}$$

whenever the equation is sound. By semantic analysis, we can show that there exist $\alpha, \beta, \gamma, \varphi, \theta \in \mathbb{R}$ and $k, \ell \in \{0, 1\}$ such that

$$\begin{aligned} \llbracket \boxed{A} \rrbracket &= \llbracket \textcircled{\alpha} \boxed{P(\varphi)} \boxed{X^k} \rrbracket & \llbracket \boxed{C} \rrbracket &= \llbracket \textcircled{\oplus} \boxed{X^k} \boxed{Z^\ell} \boxed{P(-\varphi)} \rrbracket \\ \llbracket \boxed{B} \rrbracket &= \llbracket \textcircled{\beta} \boxed{R_X(\theta)} \boxed{Z^\ell} \rrbracket & \llbracket \boxed{D} \rrbracket &= \llbracket \textcircled{\leftarrow \alpha - \beta - \gamma} \boxed{X^k} \boxed{Z^\ell} \boxed{R_X(-\theta)} \rrbracket \end{aligned}$$

where $\boxed{X^k}$ (resp. $\boxed{Z^\ell}$) denotes \boxed{X} (resp. \boxed{Z}) if $k = 1$ (resp. $\ell = 1$) and --- if $k = 0$ (resp. $\ell = 0$). Then, using the completeness of QC for one-qubit circuits (which is a direct consequence of the fact that all equations acting on at most one qubit of QC_{old} are also in QC), it

is straightforward to verify that Equations (A),(B),(25),(20),(33),(10),(9),(31),(18),(28),(D), and (27) capture all the possible cases. The details are given in Appendix C.1. ◀

► **Proposition 8.** *Equation (12) can be derived in QC.*

Proof. Using the simplification principle (Proposition 6), one can turn Equation (12) into an equivalent equation whose circuits contain only one \bigoplus . The derivation is given in Appendix C.2. We conclude the proof using the completeness of QC for circuits containing at most one CNot (Lemma 7). ◀

► **Proposition 9.** *Equation (13) can be derived in QC.*

Proof. It turns out that we can use Equation (12) to derive Equation (13) in QC. The derivation is given in Appendix C.3. ◀

► **Proposition 10.** *Equation (K_{old}^*) can be derived in QC.*

Proof. We show that for semantic reasons, we have either the angle δ_9 in (K_{old}^*) in $\{0, \pi\}$, or $\delta_2 = \delta_3 = \delta_5 = \delta_6 = 0$. When $\delta_9 = 0$, Equation (K_{old}^*) can be trivially derived from Equation (K^*). Otherwise, Equations (K^*) and (K_{old}^*) can be transformed into each other using elementary properties of multi-controlled gates. Moreover, these transformations induce a bijection between the 8-tuples of angles δ_j corresponding to the RHS of the instances of Equation (K^*) and the 9-tuples corresponding to the RHS of the instances of Equation (K_{old}^*), so that the uniqueness of the δ_j in Equation (K^*) follows from the uniqueness in Equation (K_{old}^*). Details are given in Appendix C.4. ◀

► **Theorem 11 (Completeness).** *The equational theory QC, defined in Figure 2, is complete for QC-circuits, i.e. for any QC-circuits C_1, C_2 , if $\llbracket C_1 \rrbracket = \llbracket C_2 \rrbracket$ then $\text{QC} \vdash C_1 = C_2$.*

Proof. All the rules of the complete equational theory introduced in [12] that are not in QC are provable in QC: Equations (8), (9), (10), (11) are proved in Appendix B.1, Equations (12), (13) and (K_{old}^*) are proved in Propositions 8, 9 and 10 respectively. ◀

3 Quantum circuits for isometries

In this section we consider a first standard extension of the vanilla quantum circuits which consists in allowing qubit initialisation in a specific state, namely in the $|0\rangle$ -state.

► **Definition 12.** *Let QC_{iso} be the prop generated by $\odot : 0 \rightarrow 0$, $\boxed{H} : 1 \rightarrow 1$, $\boxed{P(\varphi)} : 1 \rightarrow 1$, $\bigoplus : 2 \rightarrow 2$ and $\vdash : 0 \rightarrow 1$ for any $\varphi \in \mathbb{R}$.*

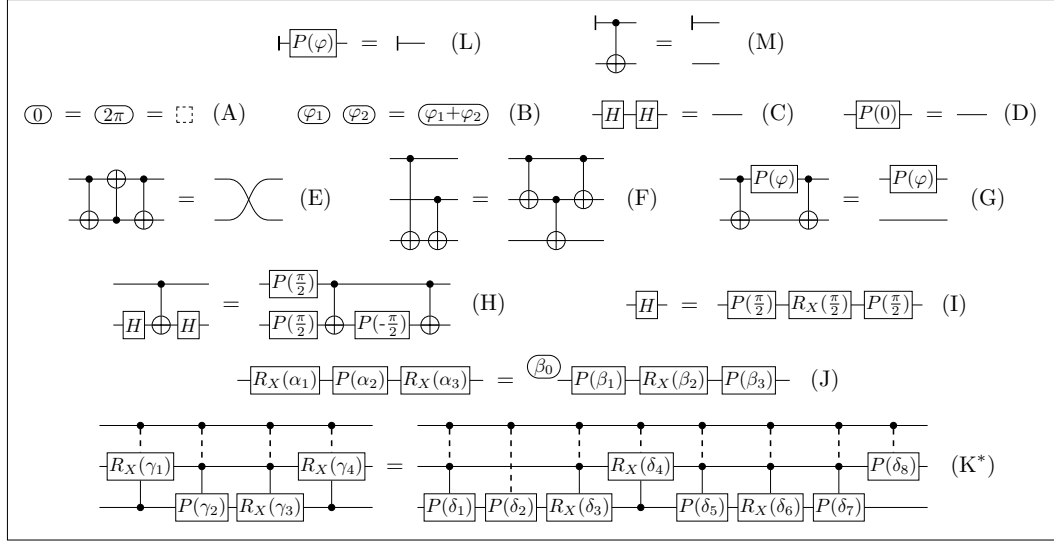
► **Definition 13 (Semantics).** *We extend the semantics $\llbracket \cdot \rrbracket$ of vanilla quantum circuits (Definition 2) with $\llbracket \vdash \rrbracket = |0\rangle$.*

► **Proposition 14 (Universality).** *Any isometry⁷ $V : \mathbb{C}^{\{0,1\}^n} \rightarrow \mathbb{C}^{\{0,1\}^m}$ can be realised by a QC_{iso} -circuit $C : n \rightarrow m$ s.t. $\llbracket C \rrbracket = V$.*

For instance, the so-called copies in the standard basis ($|x\rangle \mapsto |xx\rangle$) and in the diagonal basis can be respectively represented as follows:



⁷ An isometry is a linear map V s.t. $V^\dagger \circ V$ is the identity.



■ **Figure 4** Equational theory QC_{iso} . It contains all the equations of QC together with Equation (L) (defined for any $\varphi \in \mathbb{R}$) and Equation (M), which are new equations governing the behaviour of the new generator \vdash .

We consider the equational theory QC_{iso} , given in Figure 4, which is nothing but the equational theory QC augmented with the following two sound equations:

$$\vdash \boxed{P(\varphi)} = \vdash \quad (\text{L}) \qquad \vdash \begin{array}{c} \bullet \\ \oplus \\ \text{---} \end{array} = \vdash \quad (\text{M})$$

Viewing $\boxed{P(\varphi)}$ as a control-global-phase gate, Equations (L), (M) can be interpreted as instances of the following property: a control gate can be removed when one of its control qubit is initialised in the $|0\rangle$ -state. This kind of properties can actually be derived within QC_{iso} (see Appendix B.4).

► **Lemma 15.** *Let C be a QC_{iso} -circuit such that $\forall |\varphi\rangle \in \mathbb{C}^{2^n}$, $\llbracket C \rrbracket |\varphi\rangle = |0\rangle \otimes |\varphi\rangle$. Then:*

$$\text{QC}_{\text{iso}} \vdash \begin{array}{c} \text{---} \\ \vdots \\ \boxed{C} \\ \vdots \\ \text{---} \end{array} = \begin{array}{c} \vdash \text{---} \\ \vdots \\ \text{---} \end{array}$$

Proof. We prove that the above circuit necessarily is a QC -circuit together with a single qubit initialisation. The semantics of the QC -circuit forces it to be equivalent to a controlled circuit, which can be shown to be deletable by the qubit initialisation, thanks to Equations (L) and (M). The complete proof is in Appendix D.1. ◀

A direct corollary of Lemma 15 is the completeness of QC_{iso} for quantum circuits with at most one initialisation. Notice that one can then use Lemma 17 of [45] to essentially prove the completeness of QC_{iso} . However, as the semantics in [45] is based on CPTP maps rather than isometries (so global phases should be treated carefully), and moreover the proof of this Lemma 17 is not described, we provide a direct completeness proof of QC_{iso} in the following.

To do so, we may want to generalise Lemma 15 to any number of qubit initialisations. However, the proof does not generalise. Indeed, it relies on the fact that, semantically, the vanilla circuit of which we initialize a single qubit is necessarily of the form $\text{diag}(I, U)$, with I and U of the same dimension, so we can start with a circuit implementing U and control

each of its gates to get a circuit implementing $\text{diag}(I, U)$ with only controls and phases on the control wire. To generalise this notion to more than one qubit initialisation, where semantically we would need to implement $\text{diag}(I, U)$ with U of dimensions larger than I 's, we need a finer-grain decomposition of said matrix. We hence resort to the following unitary decomposition:

► **Lemma 16.** Let $U = \left(\begin{array}{c|c|c} I & 0 & 0 \\ \hline 0 & U_{00} & U_{01} \\ \hline 0 & U_{10} & U_{11} \end{array} \right) \left. \begin{array}{l} \}k \\ \}n-k \\ \}n \end{array} \right\} be unitary with U_{00} and U_{11} square.$

Then, there exist:

- A_0, A_1, B_0, B_1 unitary,
- $C = \text{diag}(c_1, \dots, c_d)$ and $S = \text{diag}(s_1, \dots, s_d)$ ($c_i, s_i \geq 0$ and $d \leq n - k$).

such that:

- $C^2 + S^2 = I$
- $U = \left(\begin{array}{c|c|c} I & 0 & 0 \\ \hline 0 & A_0 & 0 \\ \hline 0 & 0 & A_1 \end{array} \right) \left(\begin{array}{c|c|c|c} I & 0 & 0 & 0 \\ \hline 0 & C & 0 & -S \\ \hline 0 & 0 & I & 0 \\ \hline 0 & S & 0 & C \end{array} \right) \left(\begin{array}{c|c|c} I & 0 & 0 \\ \hline 0 & B_0 & 0 \\ \hline 0 & 0 & B_1 \end{array} \right)$

The above decomposition is a variation on the *Cosine-Sine Decomposition* (CSD) [40], which has already appeared to be useful in quantum circuit synthesis [44].

Proof. The proof itself is a variation of the proof for the usual CSD. It specifically involves the so-called RQ and SVD decompositions, which are introduced, alongside the full proof of the lemma, in Appendix D.2. ◀

It is then possible to show the completeness of QC_{iso} :

► **Theorem 17 (Completeness).** *The equational theory QC_{iso} , defined in Figure 4, is complete for QC_{iso} -circuits.*

Proof. The proof goes by showing that deriving equality between two QC_{iso} -circuits amounts to generalising Lemma 15 to any number of qubit initialisations, which is shown inductively using the above variation of the CSD. The full proof is in Appendix D.3. ◀

4 Quantum circuits with ancillae

In this section, we consider quantum circuits which are implementing unitary maps (or isometries) using ancillary qubits, a.k.a. ancillae, as additional work space. To represent quantum circuits with ancillae, we not only need to be able to initialise fresh qubits, but also to release qubits when they become useless. Note that to guarantee that the overall evolution is an isometry, one can only release a qubit in the $|0\rangle$ -state.

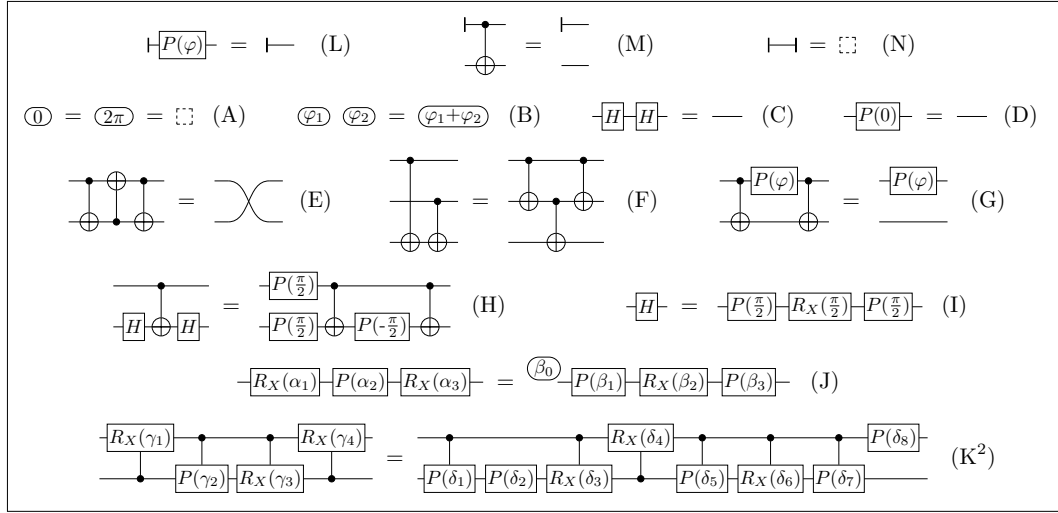
To encompass the notion of ancillary qubits we extend QC_{iso} -circuits (already equipped with qubit initialisation \vdash) with a qubit removal generator denoted \dashv . Because of the constraint that removed qubits must be in the $|0\rangle$ -state, we define the language of quantum circuits with ancillae in two steps.

► **Definition 18.** Let $\text{QC}_{\text{pre-ancilla}}$ be the prop generated by $\textcircled{\varphi} : 0 \rightarrow 0$, $\boxed{-H} : 1 \rightarrow 1$, $\boxed{-P(\varphi)} : 1 \rightarrow 1$, $\uparrow : 2 \rightarrow 2$, $\vdash : 0 \rightarrow 1$ and $\dashv : 1 \rightarrow 0$ for any $\varphi \in \mathbb{R}$.

► **Definition 19** (Semantics). We extend the semantics $\llbracket \cdot \rrbracket$ of quantum circuits for isometries (Definition 13) with $\llbracket \dashv \rrbracket = \langle 0 |$.

Notice that the semantics of a $\mathbf{QC}_{\text{pre-ancilla}}$ -circuit is not necessarily an isometry as $\llbracket \dashv \rrbracket$ is not isometric.⁸ As a consequence, we define $\mathbf{QC}_{\text{ancilla}}$ as the subclass of $\mathbf{QC}_{\text{pre-ancilla}}$ -circuits with an isometric semantics:

► **Definition 20.** Let $\mathbf{QC}_{\text{ancilla}}$ be the sub-prop of $\mathbf{QC}_{\text{pre-ancilla}}$ -circuit C such that $\llbracket C \rrbracket$ is an isometry.



■ **Figure 5** Equational theory $\mathbf{QC}_{\text{ancilla}}$. It contains all the equations of \mathbf{QC}_{iso} where Equation (K^*) has been replaced by Equation (K^2) , together with Equation (N) , which is a new equation that allows one to create ancillae.

Notice in particular that any \mathbf{QC}_{iso} -circuit is in $\mathbf{QC}_{\text{ancilla}}$, which implies the universality of $\mathbf{QC}_{\text{ancilla}}$ for isometries. We equip $\mathbf{QC}_{\text{ancilla}}$ -circuits with the equational theory $\mathbf{QC}_{\text{ancilla}}$ given in Figure 5, which is nothing but the equational theory \mathbf{QC}_{iso} where Equation (K^*) is replaced by its 2-qubit version Equation (K^2) , together with a new elementary equation (N) governing the behaviour of the qubit removal generator \dashv .

$$\dashv \dashv = \square \quad (N)$$

Quantum circuits with ancillae form a standard model of quantum computing. They are for instance used in the context of quantum oracles: given a circuit $C_f : n + 1 \rightarrow n + 1$ whose semantics is $|x, y\rangle \mapsto |x, y \oplus f(x)\rangle$ for some boolean function f , one can implement the corresponding phase oracle C'_f whose semantics is $|x\rangle \mapsto (-1)^{f(x)} |x\rangle$ as follows:

$$\dashv C'_f \dashv := \frac{\dashv C_f \dashv}{\dashv X \dashv H \dashv C_f \dashv H \dashv X \dashv}$$

⁸ Actually any linear map L s.t. $L^\dagger L \sqsubseteq I$ can be implemented by a $\mathbf{QC}_{\text{pre-ancilla}}$ -circuit, where \sqsubseteq is the Löwner partial order. Thus $\mathbf{QC}_{\text{pre-ancilla}}$ can be seen as a language for postselected quantum computations.

Proof. Proposition 22 implies that for any \dashv -free circuits C_1, C_2 , if $\mathbf{QC}_{\text{iso}} \vdash C_1 = C_2$ then $\mathbf{QC}_{\text{ancilla}} \vdash C_1 = C_2$. Using deformation of circuits, any $\mathbf{QC}_{\text{ancilla}}$ -circuit $C : n \rightarrow m$ can be written $\begin{array}{c} \vdots \\ \boxed{C'} \\ \vdots \\ \vdots \\ \vdots \end{array}$, where $C' : n \rightarrow m + k$ is a \mathbf{QC}_{iso} -circuit. Since both $\llbracket C \rrbracket$ and $\llbracket C' \rrbracket$ are isometries and $\llbracket C \rrbracket = (Id \otimes \langle 0^k |) \llbracket C' \rrbracket$, we have $\llbracket C' \rrbracket = \llbracket C \rrbracket \otimes |0^k\rangle$. Given two $\mathbf{QC}_{\text{ancilla}}$ -circuits C_1, C_2 s.t. $\llbracket C_1 \rrbracket = \llbracket C_2 \rrbracket$, let $C'_1 : n \rightarrow m + k$, and $C'_2 : n \rightarrow m + \ell$ be the corresponding \mathbf{QC}_{iso} -circuits. W.l.o.g. assume $k \leq \ell$, and pad C'_1 with $\ell - k$ qubit initialisations: $C''_1 := C'_1 \otimes (\dashv)^{\otimes \ell - k}$. We have $\llbracket C''_1 \rrbracket = \llbracket C'_2 \rrbracket$, so by completeness of \mathbf{QC}_{iso} , $\mathbf{QC}_{\text{ancilla}} \vdash C''_1 = C'_2$, so $\mathbf{QC}_{\text{ancilla}} \vdash C_1 \otimes (\dashv)^{\otimes \ell - k} = C_2$. It suffices to apply Equation (N) to obtain $\mathbf{QC}_{\text{ancilla}} \vdash C_1 = C_2$. \blacktriangleleft

5 Quantum circuits with discard for completely positive map

The last extension considered in this paper is the addition of a discard operator which consists in tracing out qubits. Contrary to quantum circuits with ancillae, any qubit can be discarded whatever its state is. Discarding a qubit is depicted by \dashv .

► **Definition 24.** Let $\mathbf{QC}_{\text{discard}}$ be the prop generated by $\boxed{H} : 1 \rightarrow 1$, $\boxed{P(\varphi)} : 1 \rightarrow 1$, $\uparrow : 2 \rightarrow 2$, $\vdash : 0 \rightarrow 1$ and $\dashv : 1 \rightarrow 0$ for any $\varphi \in \mathbb{R}$.

The ability to discard qubits implies that the evolution represented by such a circuit is not pure anymore. As a consequence the semantics is a completely positive trace-preserving (CPTP) map acting on density matrices (trace 1 positive semi-definite Hermitian matrices). Formally the new semantics is defined as follows:

► **Definition 25 (Semantics).** For any quantum $\mathbf{QC}_{\text{discard}}$ -circuit $C : n \rightarrow m$, let $\langle C \rangle : \mathcal{M}_{2^n, 2^n}(\mathbb{C}) \rightarrow \mathcal{M}_{2^m, 2^m}(\mathbb{C})$ be the semantics of C inductively defined as the linear map $\langle C_2 \circ C_1 \rangle = \langle C_2 \rangle \circ \langle C_1 \rangle$; $\langle C_1 \otimes C_2 \rangle = \langle C_1 \rangle \otimes \langle C_2 \rangle$; $\langle \dashv \rangle = \rho \mapsto \text{tr}(\rho)$ and for any other generator g , $\langle g \rangle = \rho \mapsto \llbracket g \rrbracket \rho \llbracket g \rrbracket^\dagger$, where $\text{tr}(M)$ is the trace of the matrix M and M^\dagger its adjoint.

Notice that the global phase generator \oplus is not part of the prop anymore. If it were, its interpretation would be $\langle \oplus \rangle = \rho \mapsto \llbracket \oplus \rrbracket \rho \llbracket \oplus \rrbracket^\dagger = e^{i\varphi} \rho e^{-i\varphi} = \rho$, which is the same as that of the empty circuit. Thus, for this model the X-rotation can simply be defined as $\boxed{R_X(\theta)} := \boxed{H} \boxed{P(\theta)} \boxed{H}$ (the same definition as Figure 1 but without the global phase).

► **Proposition 26 (Universality).** $\mathbf{QC}_{\text{discard}}$ is universal for CPTP maps.

Proof. According to the Stinespring dilation lemma [46], any CPTP map $F : \mathcal{M}_{2^n, 2^n}(\mathbb{C}) \rightarrow \mathcal{M}_{2^m, 2^m}(\mathbb{C})$ can be purified as an isometry $V : \mathbb{C}^{2^n} \rightarrow \mathbb{C}^{2^{m+k}}$ such that for any ρ , $F(\rho) = \text{tr}_k(V\rho V^\dagger)$, where $\text{tr}_k(\cdot)$ is the partial trace of the last k qubits. By universality of \mathbf{QC}_{iso} there exists a circuit C such that $\llbracket C \rrbracket = V$. Let C' be the global-phase-free version of C , thus $\llbracket C' \rrbracket = e^{i\theta} V$. Seen as a $\mathbf{QC}_{\text{discard}}$ -circuit, C' has the semantics $\langle C' \rangle = \rho \mapsto (e^{i\theta} V) \rho (e^{i\theta} V)^\dagger = V \rho V^\dagger$. Discarding the last k qubits of C' leads to a $\mathbf{QC}_{\text{discard}}$ -circuit implementing F . \blacktriangleleft

The new generator and new semantics allow us to model measurements. For instance, the standard basis measurement can be obtained via:



► **Theorem 27** (Completeness). *The equational theory $\text{QC}_{\text{discard}}$, defined in Figure 6, is complete for $\text{QC}_{\text{discard}}$ -circuits.*

Proof. We can use the *discard construction* [9] to build $\text{QC}_{\text{iso}}^{\text{!}}$ from QC_{iso} , by adding equation:

$$\dashv^{\otimes m} \circ U = \dashv^{\otimes n} \quad (17)$$

for any QC_{iso} -circuit $U : n \rightarrow m$. The discard construction guarantees that $\text{QC}_{\text{iso}}^{\text{!}}$ is complete for CPTP maps (Proposition 2 in [9]). It remains to prove that all equations in $\text{QC}_{\text{iso}}^{\text{!}}$ derive from those of $\text{QC}_{\text{discard}}$. All equations of the former except Equations (K*) and (17) appear in $\text{QC}_{\text{discard}}$. Those are trivially derivable. As mentioned above, it is possible to prove (K*) from $\text{QC}_{\text{discard}}$ exactly as in the case of $\text{QC}_{\text{ancilla}}$ by replacing each occurrence of $\vdash = \square$ by $\dashv = \square$. This means all the equations of $\text{QC}_{\text{iso}}^{\text{!}}$ are derivable. Finally, all the equations $\dashv^{\otimes m} \circ U = \dashv^{\otimes n}$ for different isometries U can be derived from Equations (O), (P), (Q), and (R). ◀

6 Concluding remarks

We have simplified the complete equational theory for quantum circuits, and provided ones for standard extensions of quantum circuits, including qubit initialisation, ancillae, and/or qubit discarding. The equational theory can be simplified in these more general settings, leading in particular to equations acting on a bounded number of qubits, avoiding the use of controlled gates on arbitrary number of qubits. It is interesting to notice that increasing the expressive power of the model makes the equational theory simpler.

This simplification of the equational theory is a step towards a minimal equational theory (i.e. an equational theory where each equation provably cannot be derived from the other ones). Notice that based on the present work, a minimal complete equational theory for vanilla quantum circuits has been introduced recently [10], showing in particular that equations acting on an unbounded number of qubits are necessary for vanilla quantum circuits. The question of the minimality in the context of quantum circuits with qubit initialisation, ancillae, and/or qubit discarding remains open.

Getting rid of Equation (K*) eases also the practical implementation of the rewriting rules as it avoids to consider a family of rules acting on an unbounded of qubits. Notice that regarding practical considerations, various equations presented in this paper have parameters, e.g. $\text{---}[\overline{R_X(\alpha_1)}]\text{---}[\overline{P(\alpha_2)}]\text{---}[\overline{R_X(\alpha_3)}]\text{---} = \text{---}[\overline{P(\beta_1)}]\text{---}[\overline{R_X(\beta_2)}]\text{---}[\overline{P(\beta_3)}]\text{---}$ that should be read as follows: for any angle α_i on the LHS, there exist β_j on the RHS so that the equation holds. β_j can be computed using fairly simple trigonometric operations. Notice that even if the equation looks non-symmetric, one can show conversely that for any β_j there exist α_i angles such that the equation holds (see Equation (26)).

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Appendix content

A Bullet-based graphical notation for multi-controlled gates 19

B Proofs of intermediate circuit equations 20

 B.1 Proofs of Equations (8),(9),(10) and (11) of QC_{old} 20

 B.2 Proofs of usual circuit identities 21

 B.3 Proofs of usual circuit identities over multi-controlled gates 23

 B.4 Proofs of usual circuit identities using ancillae 25

C Completeness of QC 27

 C.1 1-CNot completeness 27

 C.2 Proof of Equation (12) of QC_{old} 32

 C.3 Proof of Equation (13) of QC_{old} 33

 C.4 Proof of Equation (K^*_{old}) , existence and uniqueness of the RHS of Equation (K^*) 35

D Completeness of QC_{iso} 44

 D.1 Proof of Lemma 15 44

 D.2 Proof of Lemma 16 45

 D.3 Proof of Theorem 17 46


E Completeness of $QC_{ancilla}$ 49

 E.1 Proof of Proposition 21 49

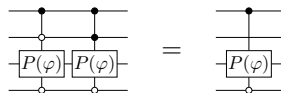
 E.2 Proof of Equation (K^3) in $QC_{ancilla}$ 51

 E.3 Proof of Equation (K^*) in $QC_{ancilla}$ 60

A Bullet-based graphical notation for multi-controlled gates

We use the standard bullet-based graphical notation for multi-controlled gates where the *negative control* (or *anti-control*) \dashv is a shortcut notation for $\boxed{X} \dashv \boxed{X}$. For instance,  stands for the gate $\boxed{P(\varphi)}$ on the third qubit positively controlled by the first and fourth qubits and negatively controlled by the second qubit. According to [12] we can simulate the expected behaviour of this bullet-based notation in QC without using Equation (K^*) .

Combining a control and anti-control on the same qubit makes the evolution independent of this qubit. This is provable in QC without (K^*) and illustrated by the following example.



Another expected behaviour provable in QC without (K^*) is the fact that controlled and anti-controlled gates commute (even if the target qubits are not the same in both gates).

This is illustrated by the two following examples.

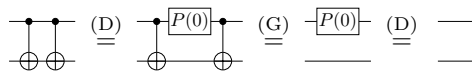


In the following, the use of such properties is denoted by (\diamond) and refers to Propositions 15, 16 and 17 (together with Propositions 10 and 11 in some cases) of [12].

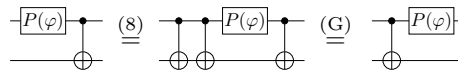
B Proofs of intermediate circuit equations

B.1 Proofs of Equations (8),(9),(10) and (11) of QC_{old}

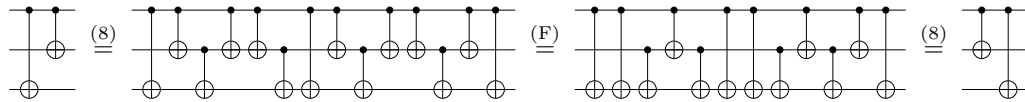
Proof of Equation (8).



Proof of Equation (9).

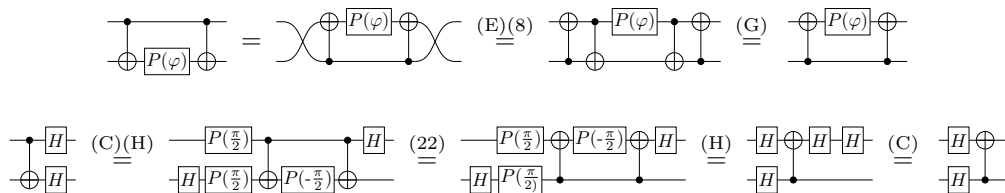


Proof of Equation (11).



$\boxed{P(\varphi_1)}\boxed{P(\varphi_2)} = \boxed{P(\varphi_1 + \varphi_2)}$ (18)	$\boxed{X}\boxed{P(\varphi)}\boxed{X} = \overset{\oplus}{P(-\varphi)}$ (19)
$\boxed{X}\boxed{X} = \text{---}$ (20)	$\boxed{P(2\pi)} = \text{---}$ (21)
(22)	(23)
	(24)

Proof of Equations (18),(19),(20),(21),(22),(23) and (24). It has been proven in Proposition 20 of [12] that Equations (18) and (19) are consequences of Equation (J) in QC_{old}. The derivations still holds in QC. Equation (20) is a direct consequence of Equations (19), (D), (A) and (B). Equation (21) is a direct consequence of Equations (20), (C) and (18). Equations (22),(23) and (24) are proved as follows.



$$\begin{aligned}
&\stackrel{(C)}{=} \overset{\alpha_0}{\text{---}} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \\
&\stackrel{(J)}{=} \overset{\alpha_0 + \beta'_0}{\text{---}} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \\
&\stackrel{(1)}{=} \overset{\beta_0}{\text{---}} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \\
&\stackrel{(C)}{=} \overset{\beta_0}{\text{---}} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---}
\end{aligned}$$

With $\alpha_0 := \frac{\alpha_1 - \alpha_2 + \alpha_3}{2}$ and $\beta_0 := \alpha_0 + \beta'_0 + \frac{\beta_1 - \beta_2 + \beta_3}{2}$. ◀

Proof of Equation (27).

$$\text{---} \text{---} \text{---} \stackrel{(1)}{=} \overset{\textcircled{1}}{\text{---}} \text{---} \text{---} \text{---} \stackrel{(D)(A)}{=} \text{---} \text{---} \text{---} \stackrel{(C)}{=} \text{---}$$

Proof of Equation (28).

$$\begin{aligned}
\text{---} \text{---} \text{---} \text{---} \text{---} \stackrel{(1)}{=} \overset{-\frac{\theta_1 - \theta_2}{2}}{\text{---}} \text{---} \text{---} \text{---} \text{---} \text{---} \stackrel{(C)}{=} \overset{-\frac{\theta_1 - \theta_2}{2}}{\text{---}} \text{---} \text{---} \text{---} \text{---} \\
\stackrel{(18)}{=} \overset{-\frac{\theta_1 + \theta_2}{2}}{\text{---}} \text{---} \text{---} \text{---} \text{---} \stackrel{(1)}{=} \text{---} \text{---} \text{---}
\end{aligned}$$

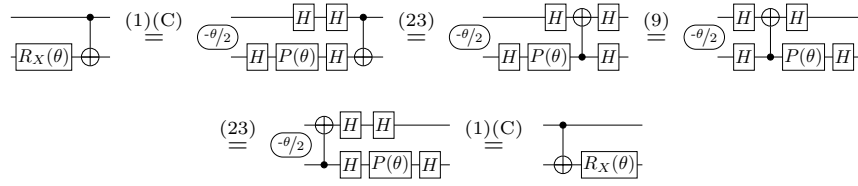
Proof of Equation (29).

$$\begin{aligned}
\text{---} \text{---} \text{---} \text{---} \text{---} \stackrel{(3)(1)}{=} \overset{-\theta/2}{\text{---}} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \stackrel{(C)}{=} \overset{-\theta/2}{\text{---}} \text{---} \text{---} \text{---} \text{---} \\
\stackrel{(19)}{=} \overset{\theta/2}{\text{---}} \text{---} \text{---} \text{---} \text{---} \stackrel{(1)}{=} \overset{\theta/2}{\text{---}} \overset{-\theta/2}{\text{---}} \text{---} \stackrel{(B)(A)}{=} \text{---} \text{---}
\end{aligned}$$

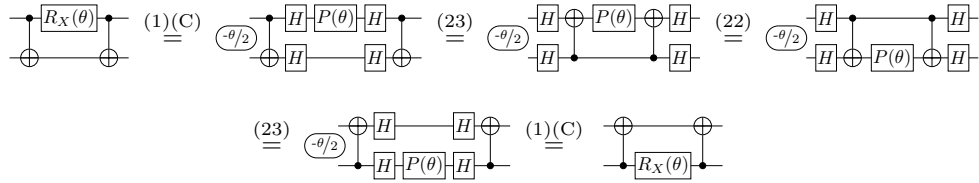
Proof of Equation (30).

$$\begin{aligned}
\text{---} \text{---} \stackrel{(D)(18)(27)(28)}{=} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \\
\stackrel{(1)}{=} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \\
\stackrel{(C)}{=} \text{---} \text{---} \text{---} \text{---} \\
\stackrel{(1)}{=} \overset{\frac{\pi}{4}}{\text{---}} \text{---} \text{---} \text{---} \text{---} \\
\stackrel{(1)}{=} \overset{\frac{\pi}{4}}{\text{---}} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \\
\stackrel{(18)(D)}{=} \overset{\frac{\pi}{4}}{\text{---}} \text{---} \text{---} \text{---}
\end{aligned}$$

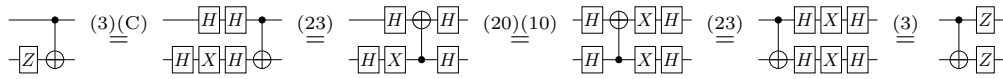
Proof of Equation (31).



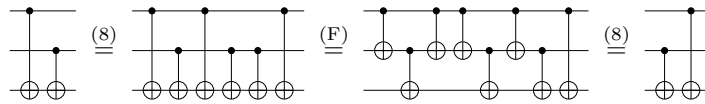
Proof of Equation (32).



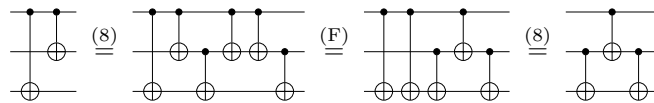
Proof of Equation (33).



Proof of Equation (34).



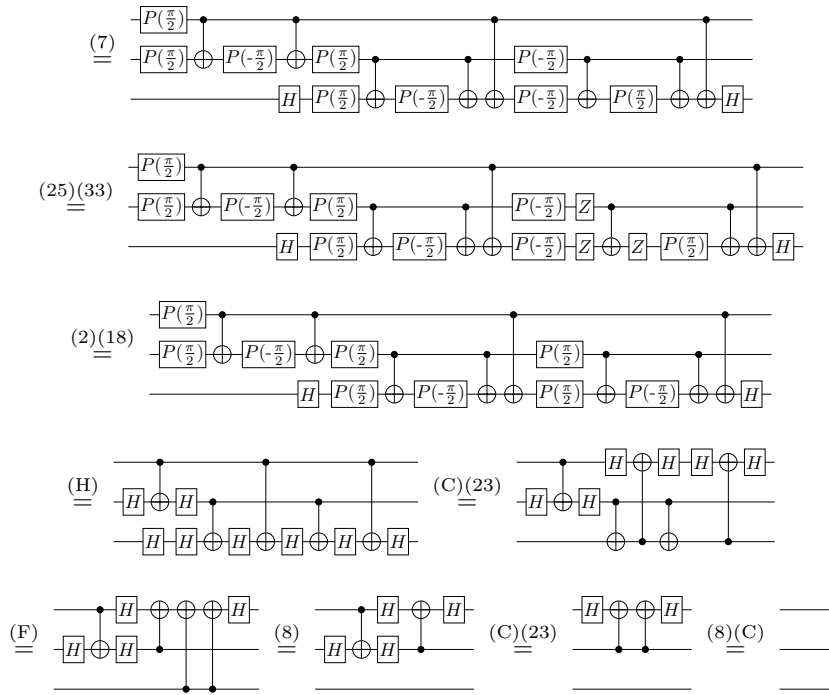
Proof of Equation (35).



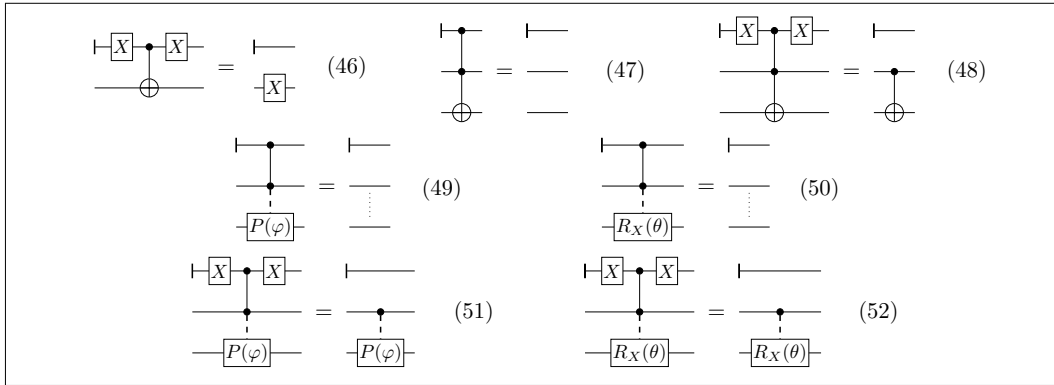
B.3 Proofs of usual circuit identities over multi-controlled gates

Proof of Equations (36),(37),(38),(39),(40),(41),(42),(43) and (44). Equations (36), (38) and (39) are proved in Proposition 13 of [12]. Equation (37) is proved in Lemma 48 of [12]. Equation (40) follows directly from Lemmas 53 and 54 of [12]. Equation (41) is proved in Lemma 47 of [12]. Equation (42) is proved in Proposition 12 of [12]. Equations (43) and (44) are proved in Proposition 11 of [12]. The proofs also hold for the equational theory QC because all the equations used are provable in QC (more precisely, one can check that that Equation (K_{old}^*) is not used, and that all the other equations of QC_{old} are provable in QC without using multi-controlled gates).

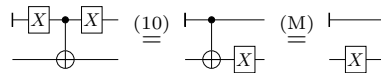




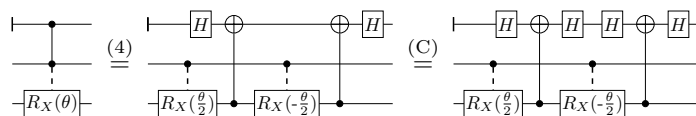
B.4 Proofs of usual circuit identities using ancillae

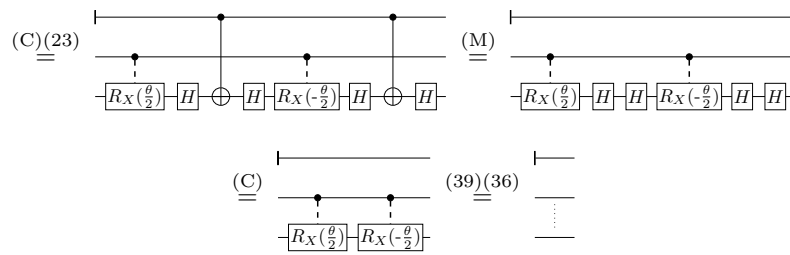


Proof of Equation (46).

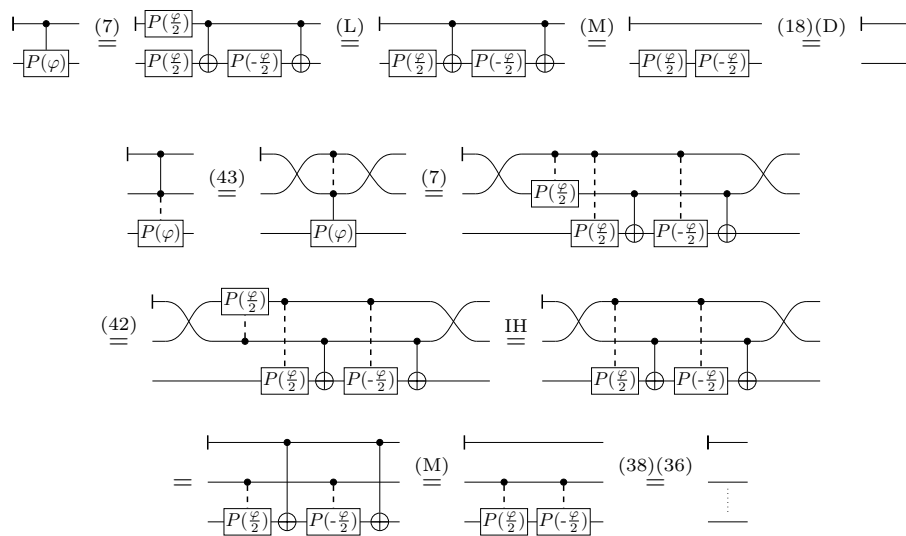


Proof of Equation (50).

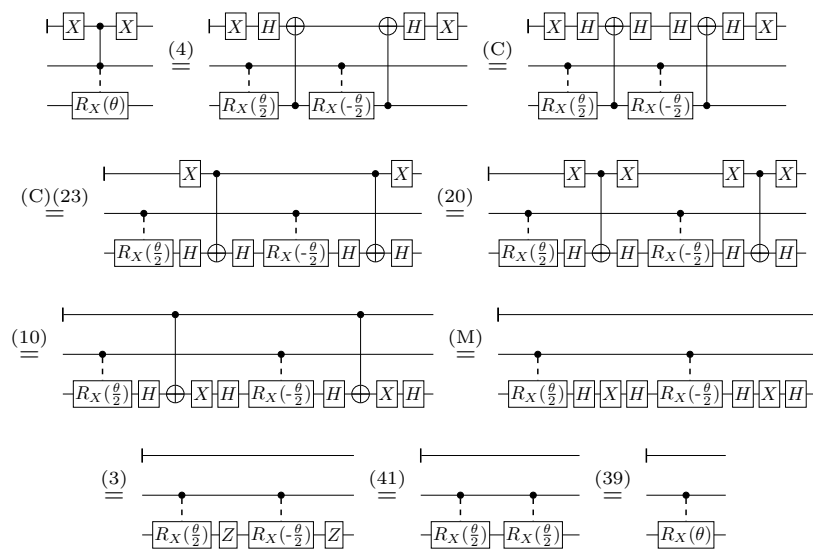




Proof of Equation (49). By induction on the number of controls with base case $n = 1$ control.



Proof of Equation (52).



Proof of Equation (51).

Proof of Equation (47).

Proof of Equation (48).

C Completeness of QC

C.1 1-CNOT completeness

In this Appendix, I , X , Z , CNOT , $P(\varphi)$ and $R_X(\theta)$ refers to the unitaries associated with the quantum gates --- , $\text{---}[X]$, $\text{---}[Z]$, $\text{---}\oplus$, $\text{---}[P(\varphi)]$ and $\text{---}[R_X(\theta)]$ respectively.

► **Lemma 28** (1-qubit completeness). *QC is complete for 1-qubit quantum circuits, i.e. for any 1-qubit QC-circuits C_1, C_2 , if $\llbracket C_1 \rrbracket = \llbracket C_2 \rrbracket$ then $\text{QC} \vdash C_1 = C_2$.*

Proof. QC contains all the equations of the complete equational theory QC_{old} acting on at most one qubit.

► **Lemma 29.** *By inputting and projecting the CNOT unitary on $|0\rangle_1, |1\rangle_1, |+\rangle_2, |-\rangle_2$ and $\langle 0|_1, \langle 1|_1, \langle +|_2, \langle -|_2$, we get the following equations:*

$$\begin{aligned} \text{CNOT } |0\rangle_1 &= (I \otimes I) |0\rangle_1 & \langle 0|_1 \text{CNOT} &= \langle 0|_1 (I \otimes I) \\ \text{CNOT } |1\rangle_1 &= (I \otimes X) |1\rangle_1 & \langle 1|_1 \text{CNOT} &= \langle 1|_1 (I \otimes X) \\ \text{CNOT } |+\rangle_2 &= (I \otimes I) |+\rangle_2 & \langle +|_2 \text{CNOT} &= \langle +|_2 (I \otimes I) \\ \text{CNOT } |-\rangle_2 &= (Z \otimes I) |-\rangle_2 & \langle -|_2 \text{CNOT} &= \langle -|_2 (Z \otimes I) \end{aligned}$$

Proof. By straightforward analysis.

► **Lemma 30.** *Let $U \in \mathcal{U}_2$ be a 1-qubit unitary. If $\langle 0|U|0\rangle = 0 \vee \langle 1|U|1\rangle = 0$ then there exist $\varphi, \delta \in \mathbb{R}$ such that $U = e^{i\delta}XP(\varphi)$. Similarly, if $\langle +|U|+\rangle = 0 \vee \langle -|U|-\rangle = 0$ then there exist $\theta, \delta \in \mathbb{R}$ such that $U = e^{i\delta}ZR_X(\theta)$.*

Proof. First notice that $\langle 0|U|0\rangle = 0$ iff $\langle 1|U|1\rangle = 0$. Then by unitarity there exists $\delta, \phi \in \mathbb{R}$ such that $U = \begin{pmatrix} 0 & e^{i\phi} \\ e^{i\delta} & 0 \end{pmatrix} = X \begin{pmatrix} e^{i\delta} & 0 \\ 0 & e^{i\phi} \end{pmatrix} = e^{i\delta} X \begin{pmatrix} 1 & 0 \\ 0 & e^{i(\phi-\delta)} \end{pmatrix}$. And we are done by taking $\varphi := \phi - \delta$.

We prove the second statement by reducing it to the first one. $\langle +|U|+\rangle = 0 \vee \langle -|U|-\rangle = 0$ iff $\langle 0|H U H|0\rangle = 0 \vee \langle 1|H U H|1\rangle = 0$. Thus there exists $\theta, \phi \in \mathbb{R}$ such that $H U H = e^{i\phi} X P(\theta)$. This implies that $U = e^{i\phi} H X P(\theta) H = e^{i(\phi+\frac{\theta}{2})} Z R_X(\theta)$ and we are done by taking $\delta := \phi + \frac{\theta}{2}$. \blacktriangleleft

► **Lemma 31.** For any $\varphi, \varphi', \delta \in \mathbb{R}$, if $P(\varphi)P(\varphi') = e^{i\delta}I$ then $\varphi' = -\varphi \pmod{2\pi}$. Similarly, for any $\theta, \theta', \delta \in \mathbb{R}$, if $R_X(\theta)R_X(\theta') = e^{i\delta}I$ then $\theta' = -\theta \pmod{2\pi}$.

Proof. For the first statement $P(\varphi)P(\varphi') = \begin{pmatrix} 1 & 0 \\ 0 & e^{i(\varphi+\varphi')} \end{pmatrix} = \begin{pmatrix} e^{i\delta} & 0 \\ 0 & e^{i\delta} \end{pmatrix} = e^{i\delta}I$ directly implies that $\varphi' = -\varphi \pmod{2\pi}$. The second statement is reduced to the first one as follows:

$$\begin{aligned} R_X(\theta)R_X(\theta') = e^{i\delta}I &\Rightarrow e^{-i(\frac{\theta}{2}+\frac{\theta'}{2})} H P(\theta) P(\theta') H = e^{i\delta}I \Rightarrow e^{-i(\frac{\theta}{2}+\frac{\theta'}{2})} P(\theta) P(\theta') = e^{i\delta}I \\ &\Rightarrow P(\theta) P(\theta') = e^{i(\delta+\frac{\theta}{2}+\frac{\theta'}{2})} I \Rightarrow \theta' = -\theta \pmod{2\pi} \end{aligned}$$

► **Lemma 32.** Let $A, B, C, D \in \mathcal{U}_2$ be 1-qubit unitaries, if $(C \otimes D) \circ \text{CNOT} \circ (A \otimes B) = \text{CNOT}$ (see the following circuit representation) then there exist $\alpha, \beta, \gamma, \varphi, \theta \in \mathbb{R}$ and $k, \ell \in \{0, 1\}$ such that $A = e^{i\alpha} X^k P(\varphi)$, $B = e^{i\beta} Z^\ell R_X(\theta)$, $C = e^{i\gamma} P(-\varphi) Z^\ell X^k$ and $D = e^{i(-\alpha-\beta-\gamma)} R_X(-\theta) Z^\ell X^k$.

$$\left[\begin{array}{c} \boxed{A} \text{---} \bullet \text{---} \boxed{C} \\ \boxed{B} \oplus \text{---} \boxed{D} \end{array} \right] = \left[\begin{array}{c} \bullet \\ \oplus \end{array} \right]$$

Proof. From the condition we derive four equations satisfied by A, B, C, D and we conduct a case distinction corresponding to the four possible assignments of $k, \ell \in \{0, 1\}$.

$$\begin{aligned} (C \otimes D) \circ \text{CNOT} \circ (A \otimes B) &= \text{CNOT} \\ &\Rightarrow \begin{cases} (C \otimes D) \circ \text{CNOT} \circ (I \otimes B) = \text{CNOT} \circ (A^\dagger \otimes I) \\ (C \otimes D) \circ \text{CNOT} \circ (A \otimes I) = \text{CNOT} \circ (I \otimes B^\dagger) \end{cases} \\ &\Rightarrow \begin{cases} \langle 0|_1 (C \otimes D) \circ \text{CNOT} \circ (I \otimes B) |0\rangle_1 = \langle 0|_1 \text{CNOT} \circ (A^\dagger \otimes I) |0\rangle_1 \\ \langle 1|_1 (C \otimes D) \circ \text{CNOT} \circ (I \otimes B) |1\rangle_1 = \langle 1|_1 \text{CNOT} \circ (A^\dagger \otimes I) |1\rangle_1 \\ \langle +|_2 (C \otimes D) \circ \text{CNOT} \circ (A \otimes I) |+\rangle_2 = \langle +|_2 \text{CNOT} \circ (I \otimes B^\dagger) |+\rangle_2 \\ \langle -|_2 (C \otimes D) \circ \text{CNOT} \circ (A \otimes I) |-\rangle_2 = \langle -|_2 \text{CNOT} \circ (I \otimes B^\dagger) |-\rangle_2 \end{cases} \\ \stackrel{\text{Lemma 29}}{\Rightarrow} &\begin{cases} \langle 0|_1 (C \otimes D) \circ (I \otimes I) \circ (I \otimes B) |0\rangle_1 = \langle 0|_1 (I \otimes I) \circ (A^\dagger \otimes I) |0\rangle_1 \\ \langle 1|_1 (C \otimes D) \circ (I \otimes X) \circ (I \otimes B) |1\rangle_1 = \langle 1|_1 (I \otimes X) \circ (A^\dagger \otimes I) |1\rangle_1 \\ \langle +|_2 (C \otimes D) \circ (I \otimes I) \circ (A \otimes I) |+\rangle_2 = \langle +|_2 (I \otimes I) \circ (I \otimes B^\dagger) |+\rangle_2 \\ \langle -|_2 (C \otimes D) \circ (Z \otimes I) \circ (A \otimes I) |-\rangle_2 = \langle -|_2 (Z \otimes I) \circ (I \otimes B^\dagger) |-\rangle_2 \end{cases} \\ &\Rightarrow \begin{cases} \langle 0|C|0\rangle DB = \langle 0|A^\dagger|0\rangle I \\ \langle 1|C|1\rangle DXB = \langle 1|A^\dagger|1\rangle X \\ \langle +|D|+\rangle CA = \langle +|B^\dagger|+\rangle I \\ \langle -|D|-\rangle CZA = \langle -|B^\dagger|-\rangle Z \end{cases} \end{aligned}$$

Case $\langle 0|A^\dagger|0\rangle \neq 0$ and $\langle +|B^\dagger|+\rangle \neq 0$. It must also be the case that $\langle 0|C|0\rangle \neq 0$ and $\langle +|D|+\rangle \neq 0$. Moreover, by unitarity of A^\dagger and B^\dagger , we also have $\langle 1|A^\dagger|1\rangle \neq 0$ and $\langle -|B^\dagger|-\rangle \neq 0$. The first equation implies $D = e^{i\delta}B^\dagger$ for some $\delta \in \mathbb{R}$, which implies that $\langle +|D|+\rangle = e^{i\delta}\langle +|B^\dagger|+\rangle$ and $\langle -|D|-\rangle = e^{i\delta}\langle -|B^\dagger|-\rangle$. Then the third equation implies $C = e^{-i\delta}A^\dagger$, which implies $\langle 1|C|1\rangle = e^{-i\delta}\langle 1|A^\dagger|1\rangle$. Hence the system becomes:

$$\begin{cases} DB = e^{i\delta}I \\ DXB = e^{i\delta}X \\ CA = e^{-i\delta}I \\ CZA = e^{-i\delta}Z \end{cases} \Rightarrow \begin{cases} CA = CZAZ \\ DB = DXBX \end{cases}$$

The first equation implies that there exist $\varphi, \alpha \in \mathbb{R}$ such that $A = e^{i\alpha}P(\varphi)$ (because $A = ZAZ$), which implies that $C = e^{i(-\delta-\alpha)}P(-\varphi)$. Similarly, the second equation implies that there exist $\theta, \beta \in \mathbb{R}$ such that $B = e^{i\beta}R_X(\theta)$ (because $B = XBX$), which implies that $D = e^{i(\delta-\beta)}R_X(-\theta)$. And we are done by tacking $k = \ell = 0$ and $\gamma := -\delta - \alpha$ which leads to $\delta - \beta = -\alpha - \beta - \gamma$.

Case $\langle 0|A^\dagger|0\rangle = 0$ and $\langle +|B^\dagger|+\rangle \neq 0$. It must also be the case that $\langle 0|C|0\rangle = 0$ and $\langle +|D|+\rangle \neq 0$. Lemma 30 implies that there exist $\varphi, \varphi', \alpha, \gamma \in \mathbb{R}$ such that $A = e^{i\alpha}XP(\varphi)$ and $C = e^{i\gamma}P(\varphi')X$. Moreover, the third equation implies $CA = e^{i\delta}I$ for some $\delta \in \mathbb{R}$, thus $e^{i(\alpha+\gamma)}P(\varphi')XXP(\varphi) = e^{i\delta}I$, which implies that $\varphi' = -\varphi \pmod{2\pi}$ (Lemma 31). Then we can use the following derivation to get a new condition satisfied by B and D .

$$\left[\begin{array}{c} \text{---} P(\varphi) \text{---} X \text{---} \bullet \text{---} X \text{---} P(-\varphi) \text{---} \\ \text{---} \text{---} B \oplus D \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \right] \stackrel{(10)}{=} \left[\begin{array}{c} \text{---} P(\varphi) \text{---} \bullet \text{---} P(-\varphi) \text{---} \\ \text{---} \text{---} B \oplus X \text{---} D \text{---} \\ \text{---} \text{---} \text{---} \end{array} \right] \stackrel{(9)(18)(D)}{=} \left[\begin{array}{c} \text{---} \bullet \text{---} \\ \text{---} \text{---} B \oplus X \text{---} D \text{---} \\ \text{---} \text{---} \text{---} \end{array} \right]$$

We get $e^{i(\alpha+\gamma)}(I \otimes DX) \circ \text{CNOT} \circ (I \otimes B) = \text{CNOT}$ from which we obtain two new equations:

$$\begin{aligned} & e^{i(\alpha+\gamma)}(I \otimes DX) \circ \text{CNOT} \circ (I \otimes B) = \text{CNOT} \\ \Rightarrow & \begin{cases} e^{i(\alpha+\gamma)} \langle 0|_1 (I \otimes DX) \circ \text{CNOT} \circ (I \otimes B) |0\rangle_1 = \langle 0|_1 \text{CNOT} |0\rangle_1 \\ e^{i(\alpha+\gamma)} \langle 1|_1 (I \otimes DX) \circ \text{CNOT} \circ (I \otimes B) |1\rangle_1 = \langle 1|_1 \text{CNOT} |1\rangle_1 \end{cases} \\ \stackrel{\text{Lemma 29}}{\Rightarrow} & \begin{cases} e^{i(\alpha+\gamma)} \langle 0|_1 (I \otimes DX) \circ (I \otimes I) \circ (I \otimes B) |0\rangle_1 = \langle 0|_1 (I \otimes I) |0\rangle_1 \\ e^{i(\alpha+\gamma)} \langle 1|_1 (I \otimes DX) \circ (I \otimes X) \circ (I \otimes B) |1\rangle_1 = \langle 1|_1 (I \otimes X) |1\rangle_1 \end{cases} \\ \Rightarrow & \begin{cases} e^{i(\alpha+\gamma)}DXB = I \\ e^{i(\alpha+\gamma)}DXXB = X \end{cases} \end{aligned}$$

This implies that $DXB = DBX$, thus there exist $\theta, \beta \in \mathbb{R}$ such that $B = e^{i\beta}R_X(\theta)$ (because $B = XBX$). The first equation implies $D = e^{i(-\alpha-\beta-\gamma)}R_X(-\theta)X$, and we are done by tacking $k = 1$ and $\ell = 0$.

Case $\langle 0|A^\dagger|0\rangle \neq 0$ and $\langle +|B^\dagger|+\rangle = 0$. It must also be the case that $\langle 0|C|0\rangle \neq 0$ and $\langle +|D|+\rangle = 0$. Lemma 30 implies that there exist $\theta, \theta', \beta, \sigma \in \mathbb{R}$ such that $B = e^{i\beta}ZR_X(\theta)$ and $D = e^{i\sigma}R_X(\theta')Z$. Moreover, the first equation implies $DB = e^{i\delta}I$ for some $\delta \in \mathbb{R}$, thus $e^{i(\beta+\sigma)}R_X(\theta')ZZR_X(\theta) = e^{i\delta}I$, which implies that $\theta' = -\theta \pmod{2\pi}$ (Lemma 31). Then we can use the following derivation to get a new condition satisfied by A and C .

$$\left[\begin{array}{c} \text{---} A \text{---} \bullet \text{---} C \text{---} \\ \text{---} \text{---} R_X(\theta) \text{---} Z \oplus Z \text{---} R_X(-\theta) \text{---} \\ \text{---} \text{---} \text{---} \end{array} \right] \stackrel{(33)}{=} \left[\begin{array}{c} \text{---} A \text{---} \bullet \text{---} Z \text{---} C \text{---} \\ \text{---} \text{---} R_X(\theta) \text{---} \oplus R_X(-\theta) \text{---} \\ \text{---} \text{---} \text{---} \end{array} \right] \stackrel{(31)(28)(27)}{=} \left[\begin{array}{c} \text{---} A \text{---} \bullet \text{---} Z \text{---} C \text{---} \\ \text{---} \text{---} \oplus \text{---} \\ \text{---} \text{---} \text{---} \end{array} \right]$$

We get $e^{i(\beta+\sigma)}(CZ \otimes I) \circ \text{CNOT} \circ (A \otimes I) = \text{CNOT}$ from which we obtain two new equations:

$$e^{i(\beta+\sigma)}(CZ \otimes I) \circ \text{CNOT} \circ (A \otimes I) = \text{CNOT}$$

$$\begin{aligned}
&\Rightarrow \begin{cases} e^{i(\beta+\sigma)} \langle +|_2 (CZ \otimes I) \circ \text{CNOT} \circ (A \otimes I) |+\rangle_2 = \langle +|_2 \text{CNOT} |+\rangle_2 \\ e^{i(\beta+\sigma)} \langle -|_2 (CZ \otimes I) \circ \text{CNOT} \circ (A \otimes I) |-\rangle_2 = \langle -|_2 \text{CNOT} |-\rangle_2 \end{cases} \\
&\Rightarrow \begin{cases} e^{i(\beta+\sigma)} \langle +|_2 (CZ \otimes I) \circ (I \otimes I) \circ (A \otimes I) |+\rangle_2 = \langle +|_2 (I \otimes I) |+\rangle_2 \\ e^{i(\beta+\sigma)} \langle -|_2 (CZ \otimes I) \circ (Z \otimes I) \circ (A \otimes I) |-\rangle_2 = \langle -|_2 (Z \otimes I) |-\rangle_2 \end{cases} \\
&\Rightarrow \begin{cases} e^{i(\beta+\sigma)} CZA = I \\ e^{i(\beta+\sigma)} CZZA = Z \end{cases}
\end{aligned}$$

This implies that $CZA = CAZ$, thus there exist $\varphi, \alpha \in \mathbb{R}$ such that $A = e^{i\alpha}P(\varphi)$ (because $A = ZAZ$). The first equation implies $C = e^{i(-\alpha-\beta-\sigma)}P(-\varphi)Z$, and we are done by tacking $k = 0, \ell = 1$ and $\gamma := -\alpha - \beta - \sigma$, which leads to $\sigma = -\alpha - \beta - \gamma$.

Case $\langle 0|A^\dagger|0\rangle = 0$ and $\langle +|B^\dagger|+\rangle = 0$. It must also be the case that $\langle 0|C|0\rangle = 0$ and $\langle +|D|+\rangle = 0$. Lemma 30 implies that there exist $\varphi, \varphi', \theta, \theta', \alpha, \beta, \gamma, \delta \in \mathbb{R}$ such that $A = e^{i\alpha}XP(\varphi)$, $B = e^{i\beta}ZR_X(\theta)$, $C = e^{i\gamma}P(\varphi')X$ and $D = e^{i\delta}R_X(\theta')Z$. Then we can use the following derivation to get a new condition satisfied by $\varphi, \varphi', \theta, \theta'$.

$$\left[\begin{array}{c} \overline{\alpha+\beta+\gamma+\delta} \quad \overline{P(\varphi)} \quad \overline{X} \quad \overline{X} \quad \overline{P(\varphi')} \\ \overline{R_X(\theta)} \quad \overline{Z} \quad \oplus \quad \overline{Z} \quad \overline{R_X(\theta')} \end{array} \right] \stackrel{(10)(33)}{=} \left[\begin{array}{c} \overline{\alpha+\beta+\gamma+\delta} \quad \overline{P(\varphi)} \quad \overline{Z} \quad \overline{P(\varphi')} \\ \overline{R_X(\theta)} \quad \oplus \quad \overline{X} \quad \overline{R_X(\theta')} \end{array} \right]$$

We get $e^{i(\alpha+\beta+\gamma+\delta)}(P(\varphi')Z \otimes R_X(\theta')X) \circ \text{CNOT} \circ (P(\varphi) \otimes R_X(\theta)) = \text{CNOT}$ from which we obtain two new equations:

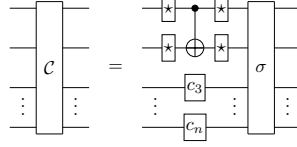
$$\begin{aligned}
&e^{i(\alpha+\beta+\gamma+\delta)}(P(\varphi')Z \otimes R_X(\theta')X) \circ \text{CNOT} \circ (P(\varphi) \otimes R_X(\theta)) = \text{CNOT} \\
&\Rightarrow \begin{cases} e^{i(\alpha+\beta+\gamma+\delta)} \langle 0|_1 (P(\varphi')Z \otimes R_X(\theta')X) \text{CNOT} (P(\varphi) \otimes R_X(\theta)) |0\rangle_1 = \langle 0|_1 \text{CNOT} |0\rangle_1 \\ e^{i(\alpha+\beta+\gamma+\delta)} \langle +|_2 (P(\varphi')Z \otimes R_X(\theta')X) \text{CNOT} (P(\varphi) \otimes R_X(\theta)) |+\rangle_2 = \langle +|_2 \text{CNOT} |+\rangle_2 \end{cases} \\
&\Rightarrow \begin{cases} e^{i(\alpha+\beta+\gamma+\delta)} \langle 0|_1 (P(\varphi')Z \otimes R_X(\theta')X) (I \otimes I) (P(\varphi) \otimes R_X(\theta)) |0\rangle_1 = \langle 0|_1 (I \otimes I) |0\rangle_1 \\ e^{i(\alpha+\beta+\gamma+\delta)} \langle +|_2 (P(\varphi')Z \otimes R_X(\theta')X) (I \otimes I) (P(\varphi) \otimes R_X(\theta)) |+\rangle_2 = \langle +|_2 (I \otimes I) |+\rangle_2 \end{cases} \\
&\Rightarrow \begin{cases} e^{i(\alpha+\beta+\gamma+\delta)} R_X(\theta') X R_X(\theta) = I \\ e^{i(\alpha+\beta+\gamma+\delta)} e^{-i(\theta+\theta')/2} P(\varphi') Z P(\varphi) = I \end{cases} \\
&\Rightarrow \begin{cases} R_X(\theta') = e^{-i(\alpha+\beta+\gamma+\delta)} R_X(-\theta) X \\ P(\varphi') = e^{-i(\alpha+\beta+\gamma+\delta)} e^{i(\theta+\theta')/2} P(-\varphi) Z \end{cases} \\
&\Rightarrow \begin{cases} R_X(\theta') = e^{-i(\alpha+\beta+\gamma+\delta)} e^{i\pi/2} R_X(\pi - \theta) \\ P(\varphi') = e^{-i(\alpha+\beta+\gamma+\delta)} e^{i(\theta+\theta')/2} P(\pi - \varphi) \end{cases} \\
&\stackrel{\text{Lemma 31}}{\Rightarrow} \begin{cases} \theta' = \pi - \theta \pmod{2\pi} \\ \varphi' = \pi - \varphi \pmod{2\pi} \end{cases}
\end{aligned}$$

Hence, we get $A = e^{i\alpha}XP(\varphi)$, $B = e^{i\beta}ZR_X(\theta)$, $C = e^{i\gamma}P(\pi - \varphi)X = e^{i\gamma}P(-\varphi)ZX$ and $D = e^{i(-\alpha-\beta-\gamma+\pi/2)}R_X(\pi - \theta)Z = e^{i(-\alpha-\beta-\gamma)}R_X(-\theta)ZX$. Thus we are done by taking $k = \ell = 1$. \blacktriangleleft

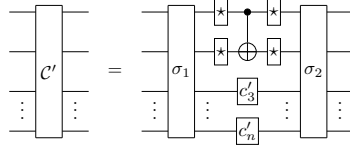
Proof of Lemma 7 (1-CNot completeness). Let $\mathcal{C}, \mathcal{C}'$ be two 1-CNot QC-circuits, i.e. circuits containing at most one $\overline{\oplus}$ gate each, such that $\llbracket \mathcal{C} \rrbracket = \llbracket \mathcal{C}' \rrbracket$.

First notice that if both $\mathcal{C}, \mathcal{C}'$ contains no CNot, then, according to Lemma 28 we have $\text{QC} \vdash \mathcal{C} = \mathcal{C}'$. If \mathcal{C} contains a CNot then one can show that \mathcal{C}' must contain a CNot otherwise they would not have the same semantics.

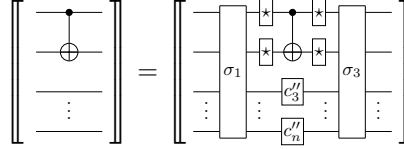
Then, w.l.o.g. we can suppose that the CNot is applied to the first two qubits in \mathcal{C} . We first show that the CNot is also applied to the first two qubits in \mathcal{C}' , and that the permutation of wires is the same in both circuits. Pushing all swaps to the right in \mathcal{C} , we get:



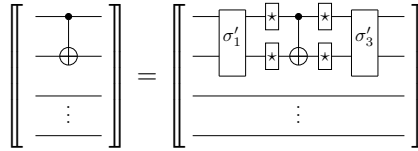
where σ is a permutation of wires. In \mathcal{C}' , using the prop equations to move the CNot on the first two qubits, we get:



By applying the inverse of all 1-qubit unitaries from \mathcal{C} , as well as the inverse of σ , $\llbracket \mathcal{C} \rrbracket = \llbracket \mathcal{C}' \rrbracket$ becomes equivalent to:



with $\sigma_3 = \sigma_2 \circ \sigma^{-1}$. It then becomes apparent that if $\sigma_1(i) \geq 3$, then $\sigma_3(\sigma_1(i)) = i$. Moreover, we get $\llbracket c_i'' \rrbracket = \llbracket - \rrbracket$. We then have:



Getting back to \mathcal{C} and \mathcal{C}' , we conclude that qubits that are not involved with the CNot have the same 1-qubit unitary applied to them on both sides, and are permuted with the rest in the same way. By completeness of QC for 1-qubit unitaries, it is now enough to show the result when \mathcal{C} and \mathcal{C}' are 2-qubit circuits.

We can now show that if a swap appears on one side, it also appears on the other side (i.e. that $\sigma'_1 = \sigma'_3$ above). Indeed, suppose that \mathcal{C} has a swap and \mathcal{C}' does not. Using the prop equations, we can push the swap to the right, and get $\mathcal{C} = \bowtie \circ \bar{\mathcal{C}}'$. Thus $\llbracket \mathcal{C} \rrbracket = \llbracket \mathcal{C}' \rrbracket$ is then equivalent to $\llbracket \bowtie \rrbracket = \llbracket \mathcal{C}' \circ \bar{\mathcal{C}}' \rrbracket$. We hence have a circuit $\mathcal{C}' \circ \bar{\mathcal{C}}'$ that implements \bowtie , using at most two CNOTs. This contradicts Theorem 6 of [48] that proves that the swap requires at least 3 CNOTs. Hence, if \mathcal{C} has a swap then so does \mathcal{C}' .

In the case where the two circuits have a swap, the equality between the two becomes equivalent (Proposition 6) to the equality without swaps on both side. Hence, we can assume w.l.o.g. that \mathcal{C} and \mathcal{C}' are 2-qubit circuits containing one and only one CNot and no swap. Moreover thanks to Equation (23) we can assume:

$$\llbracket \mathcal{C} \rrbracket = \begin{array}{|c|} \hline \boxed{A_1} \\ \hline \boxed{B_1} \oplus \boxed{D_1} \\ \hline \end{array} \begin{array}{|c|} \hline \boxed{C_1} \\ \hline \end{array} \quad \llbracket \mathcal{C}' \rrbracket = \begin{array}{|c|} \hline \boxed{A_2} \\ \hline \boxed{B_2} \oplus \boxed{D_2} \\ \hline \end{array} \begin{array}{|c|} \hline \boxed{C_2} \\ \hline \end{array}$$

for some 1-qubit circuits $\boxed{A_i}$, $\boxed{B_i}$, $\boxed{C_i}$, $\boxed{D_i}$.

First, by the simplification principle (Proposition 6), we reduce it to showing the following equation for any semantically correct 1-qubit circuits \boxed{A} , \boxed{B} , \boxed{C} , \boxed{D} .

$$\begin{array}{c} \boxed{A} \bullet \boxed{C} \\ \boxed{B} \oplus \boxed{D} \end{array} = \begin{array}{c} \bullet \\ \oplus \end{array}$$

Lemma 32 and Lemma 28 together with Equations (A) and (B) implies that this is always the case that this equation is equivalent (Proposition 6) to one of the following equations:

$$\begin{array}{ccc} \begin{array}{c} \boxed{P(\varphi)} \bullet \boxed{P(-\varphi)} \\ \boxed{R_X(\theta)} \oplus \boxed{R_X(-\theta)} \end{array} = \begin{array}{c} \bullet \\ \oplus \end{array} & \begin{array}{c} \boxed{P(\varphi)} \boxed{X} \bullet \boxed{X} \boxed{P(-\varphi)} \\ \boxed{R_X(\theta)} \oplus \boxed{X} \boxed{R_X(-\theta)} \end{array} = \begin{array}{c} \bullet \\ \oplus \end{array} \\ \begin{array}{c} \boxed{P(\varphi)} \bullet \boxed{Z} \boxed{P(-\varphi)} \\ \boxed{R_X(\theta)} \boxed{Z} \oplus \boxed{Z} \boxed{R_X(-\theta)} \end{array} = \begin{array}{c} \bullet \\ \oplus \end{array} & \begin{array}{c} \boxed{P(\varphi)} \boxed{X} \bullet \boxed{X} \boxed{Z} \boxed{P(-\varphi)} \\ \boxed{R_X(\theta)} \boxed{Z} \oplus \boxed{X} \boxed{Z} \boxed{R_X(-\theta)} \end{array} = \begin{array}{c} \bullet \\ \oplus \end{array} \end{array}$$

We conclude the proof by observing that we can derive all those equations for any $\varphi, \theta \in \mathbb{R}$ using Equations (33),(10),(9),(31),(18),(28),(D), and (27). \blacktriangleleft

C.2 Proof of Equation (12) of QC_{old}

Proof of Equation (12). We first show that any circuits (containing four CNot gates) of the form $\begin{array}{c} \oplus \oplus \oplus \oplus \\ \boxed{C_1} \bullet \boxed{C_2} \bullet \boxed{C_3} \bullet \boxed{C_4} \bullet \boxed{C_5} \end{array}$ can always be transformed in QC into a circuit (containing

only two CNot gates) of the form $\begin{array}{c} \oplus \oplus \\ \boxed{C_6} \bullet \boxed{C_7} \bullet \boxed{C_8} \end{array}$ where $\boxed{C_i}$ denotes a one-qubit circuit.

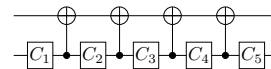
This uses the fact (referenced (*) below) that any one-qubit circuit can be transformed in QC into a circuit of the form $\overset{\alpha_0}{\boxed{R_X(\alpha_1)} \boxed{P(\alpha_2)} \boxed{R_X(\alpha_3)}}$ or $\overset{\beta_0}{\boxed{P(\beta_1)} \boxed{R_X(\beta_2)} \boxed{P(\beta_3)}}$ (by the completeness of QC for one-qubit circuits and the well-know Euler-decomposition). The derivation goes as follows.

$$\begin{array}{l} \begin{array}{c} \oplus \oplus \oplus \oplus \\ \boxed{C_1} \bullet \boxed{C_2} \bullet \boxed{C_3} \bullet \boxed{C_4} \bullet \boxed{C_5} \end{array} \\ \stackrel{(*)}{=} \begin{array}{c} \oplus \oplus \oplus \oplus \\ \overset{\alpha_0 + \beta_0}{\boxed{C_1}} \bullet \boxed{P(\alpha_1)} \boxed{R_X(\alpha_2)} \boxed{P(\alpha_3)} \bullet \boxed{C_3} \bullet \boxed{P(\beta_1)} \boxed{R_X(\beta_2)} \boxed{P(\beta_3)} \bullet \boxed{C_5} \end{array} \\ \stackrel{(9)}{=} \begin{array}{c} \oplus \oplus \oplus \oplus \\ \overset{\alpha_0 + \beta_0}{\boxed{C_1}} \bullet \boxed{P(\alpha_1)} \bullet \boxed{R_X(\alpha_2)} \bullet \boxed{P(\alpha_3)} \bullet \boxed{C_3} \bullet \boxed{P(\beta_1)} \bullet \boxed{R_X(\beta_2)} \bullet \boxed{P(\beta_3)} \bullet \boxed{C_5} \end{array} \\ \stackrel{(*)}{=} \begin{array}{c} \oplus \oplus \oplus \oplus \\ \overset{\alpha_0 + \beta_0 + \gamma_0}{\boxed{C_1}} \bullet \boxed{P(\alpha_1)} \bullet \boxed{R_X(\alpha_2)} \bullet \boxed{R_X(\gamma_1)} \bullet \boxed{P(\gamma_2)} \bullet \boxed{R_X(\gamma_3)} \bullet \boxed{R_X(\beta_2)} \bullet \boxed{P(\beta_3)} \bullet \boxed{C_5} \end{array} \\ \stackrel{(32)(31)}{=} \begin{array}{c} \oplus \oplus \oplus \oplus \\ \overset{\alpha_0 + \beta_0 + \gamma_0}{\boxed{C_1}} \bullet \boxed{P(\alpha_1)} \bullet \boxed{R_X(\gamma_1)} \bullet \boxed{R_X(\alpha_2)} \bullet \boxed{P(\gamma_2)} \bullet \boxed{R_X(\beta_2)} \bullet \boxed{R_X(\gamma_3)} \bullet \boxed{P(\beta_3)} \bullet \boxed{C_5} \end{array} \\ \stackrel{(G)}{=} \begin{array}{c} \oplus \oplus \oplus \oplus \\ \overset{\alpha_0 + \beta_0 + \gamma_0}{\boxed{C_1}} \bullet \boxed{P(\alpha_1)} \bullet \boxed{R_X(\gamma_1)} \bullet \boxed{R_X(\alpha_2)} \bullet \boxed{P(\gamma_2)} \bullet \boxed{R_X(\beta_2)} \bullet \boxed{R_X(\gamma_3)} \bullet \boxed{P(\beta_3)} \bullet \boxed{C_5} \end{array} \end{array}$$

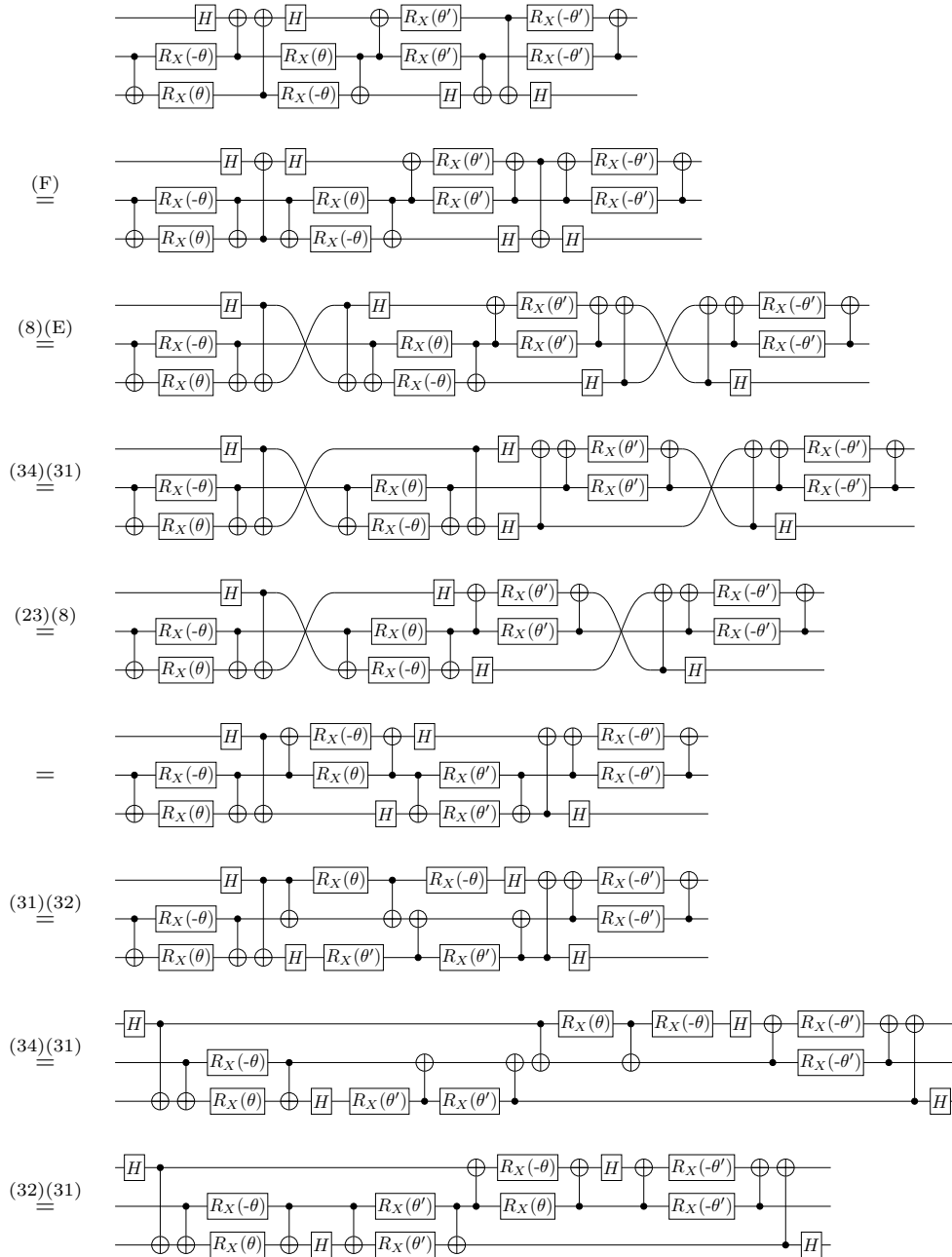
Then, using Equations (31) and (32), Equation (12) becomes

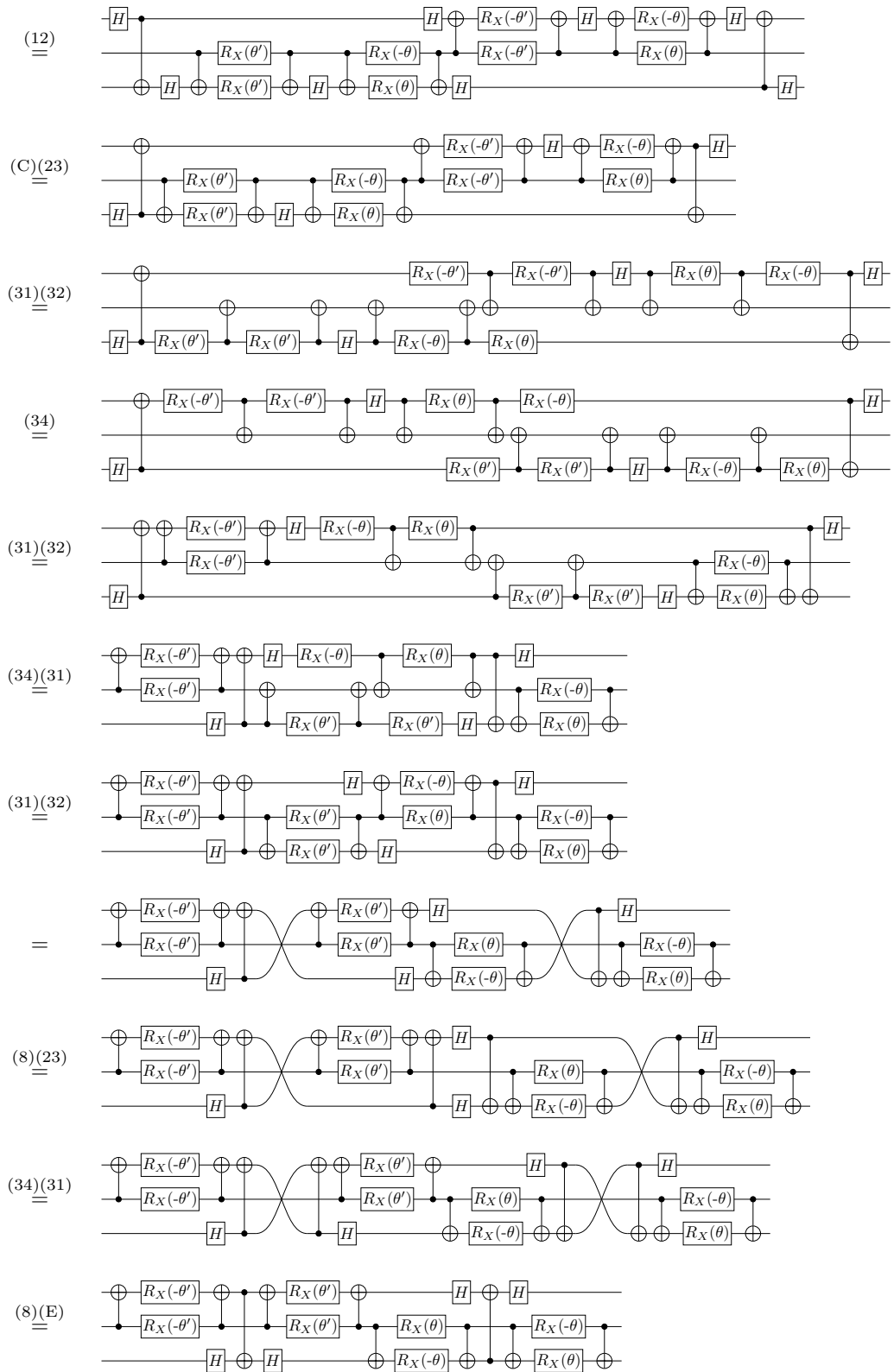
$$\begin{array}{c} \oplus \oplus \oplus \oplus \\ \boxed{R_X(\theta)} \bullet \boxed{R_X(-\theta)} \bullet \boxed{H} \bullet \boxed{R_X(\theta')} \bullet \boxed{R_X(\theta')} \bullet \boxed{H} \end{array} = \begin{array}{c} \oplus \oplus \oplus \oplus \\ \boxed{H} \bullet \boxed{R_X(\theta')} \bullet \boxed{R_X(\theta')} \bullet \boxed{H} \bullet \boxed{R_X(-\theta)} \bullet \boxed{R_X(\theta)} \end{array}$$

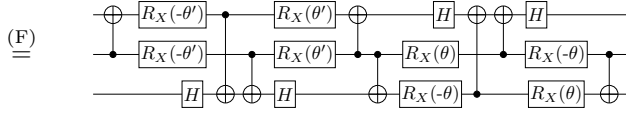
We can then use the above derivation to transform both circuits into circuits of the form $\begin{array}{c} \oplus \oplus \\ \boxed{C_6} \bullet \boxed{C_7} \bullet \boxed{C_8} \end{array}$. Then, by using the simplification principle (Proposition 6), we

can push the RHS circuit to the end of the LHS circuit, which leads to a circuit of the form  (up to a global phase) from which we can apply again the above derivation, leading to a circuit containing only two CNot gates. Then, by using the simplification principle again, we can turn the equation into an equivalent equations with only one CNot on both sides. Finally, the completeness of QC for circuits containing at most one CNot gate (Lemma 7) concludes the proof. ◀

C.3 Proof of Equation (13) of QC_{old}





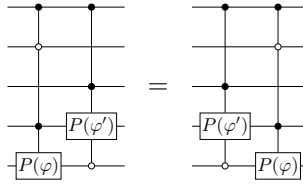


C.4 Proof of Equation (K_{old}^*) , existence and uniqueness of the RHS of Equation (K^*)

The proof uses some properties of multi-controlled gates:

► **Lemma 33.** *It follows from the equations of QC without Equation (K^*) that two multi-controlled P gates always commute, regardless of the colours and positions of their controls, and of the positions of their targets.*

For instance,



Proof of Lemma 33. This is a direct consequence of the results of [12], namely of Lemma 54 together with Propositions 11, 12 and 15. ◀

► **Lemma 34.** *The following equation is a consequence of the equations of QC:*

$$\begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{P(2\pi)} \end{array} = \begin{array}{c} \vdots \\ \vdots \\ \vdots \end{array} \quad (53)$$

► **Lemma 35.** *The following equations are consequences of the equations of QC without Equation (K^*) , together with Equation (53):*

$$\begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{R_X(2\pi)} \end{array} = \begin{array}{c} \bullet \\ \hline \boxed{P(\pi)} \end{array} \quad (54)$$

$$\begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{P(\pi)} \end{array} \begin{array}{c} \bullet \\ \hline \boxed{R_X(\theta)} \end{array} = \begin{array}{c} \bullet \\ \hline \boxed{P(\pi)} \end{array} \begin{array}{c} \bullet \\ \hline \boxed{R_X(2\pi-\theta)} \end{array} \quad (55)$$

Proof of Equation (53). The case with zero controls is a direct consequence of Equations (2), (18), and (25). For the case with one or more controls, it suffices to remark that the derivation given in [12] does not need δ_9 :

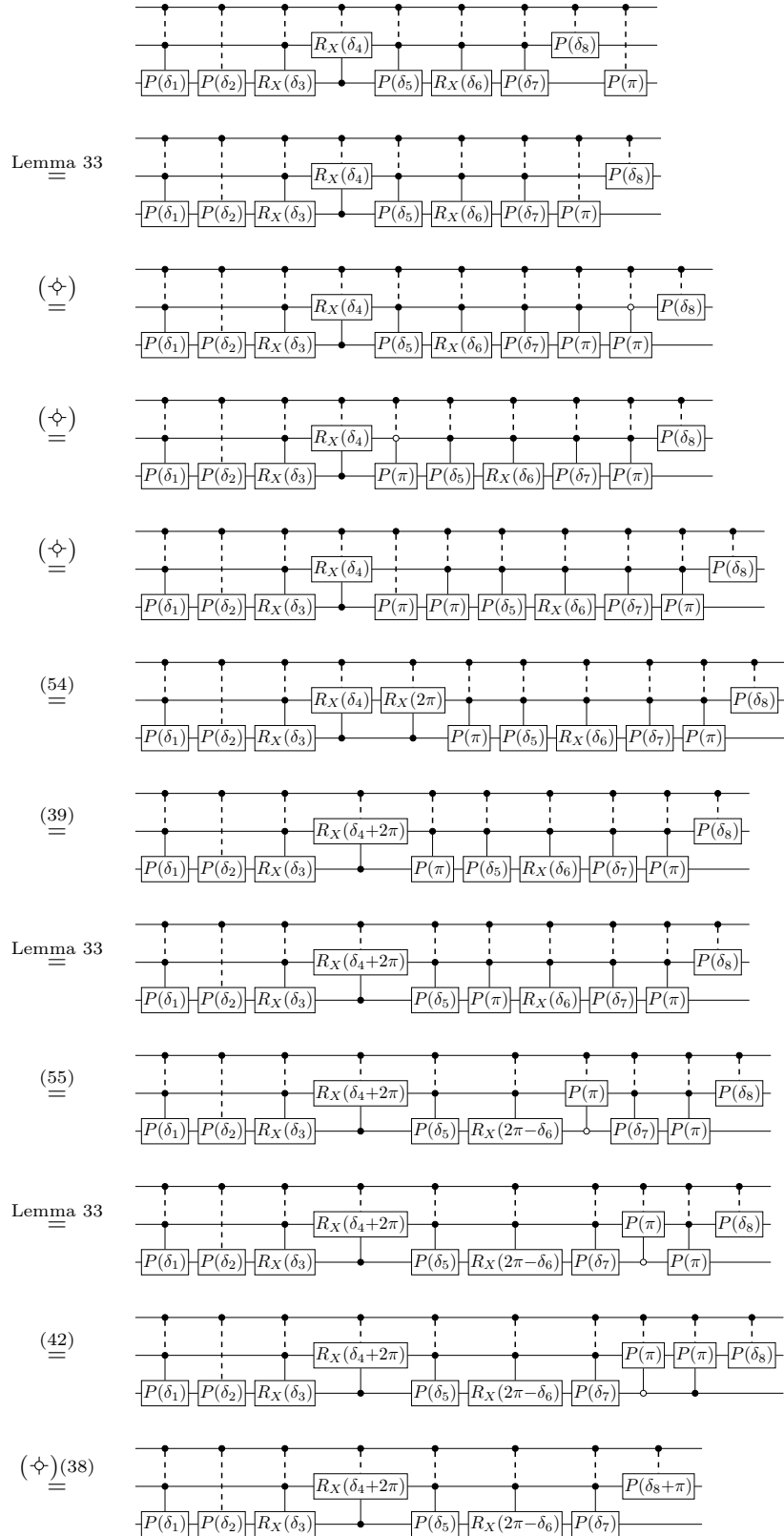
$$\begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{P(2\pi)} \end{array} \stackrel{(36)}{=} \begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{R_X(0)} \end{array} \begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{P(2\pi)} \end{array} \begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{R_X(0)} \end{array} \quad (36)$$

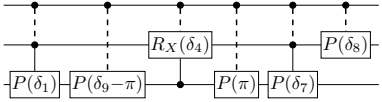
$$\stackrel{(K^*)}{=} \begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{P(0)} \end{array} \begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{P(0)} \end{array} \begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{R_X(0)} \end{array} \begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{P(0)} \end{array} \begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{R_X(0)} \end{array} \begin{array}{c} \bullet \\ \vdots \\ \bullet \\ \hline \boxed{P(0)} \end{array} \quad (K^*)$$

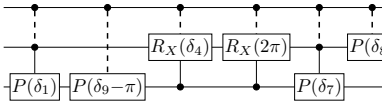
$$\stackrel{(36)}{=} \begin{array}{c} \vdots \\ \vdots \\ \vdots \end{array} \quad (36)$$

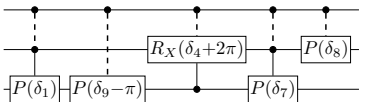
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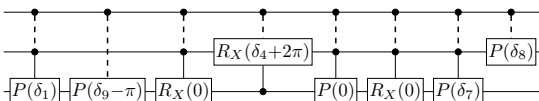
– If $\delta_9 = \pi$ and $\delta_6 \neq 0$, then



Lemma 33,
(37) 

(54) 

(39) 

(36) 

■ If $\sin(\frac{\gamma_4}{2}) = 0$, then $\cos(\frac{\gamma_4}{2}) \in \{-1, 1\}$ and one has

$$\langle 1\dots 101 | \left[\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right] | 1\dots 101 \rangle = \pm \cos\left(\frac{\gamma_1}{2}\right)$$

while, since $\delta_2 = 0$,

$$\langle 1\dots 101 | \left[\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right] | 1\dots 101 \rangle = e^{i\delta_9} \cos\left(\frac{\delta_4}{2}\right).$$

- * If $\cos(\frac{\delta_4}{2}) \neq 0$, then this implies that $e^{i\delta_9}$ is a real number, so that $\delta_9 \in \{0, \pi\}$ and we can proceed as in the first case (where $\sin(\frac{\delta_3}{2}) \sin(\frac{\delta_4}{2}) \neq 0$).
- * If $\cos(\frac{\delta_4}{2}) = 0$, then on the one hand, since $\delta_4 \in [0, 2\pi)$, one has $\delta_4 = \pi$. In turn, since $\delta_3 = 0$, the conditions of Equation (K_{old}^*) imply that $\delta_1 = 0$. On the other hand, $\cos(\frac{\gamma_1}{2}) = 0$ too, so that $\sin(\frac{\gamma_1}{2}) \in \{-1, 1\}$ and

$$\langle 1\dots 101 | \left[\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right] | 1\dots 111 \rangle = \pm i$$

while, since $\delta_2 = 0$,

$$\langle 1\dots 101 | \left[\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right] | 1\dots 111 \rangle = \pm i e^{i\delta_9}.$$

Hence, $\delta_9 \in \{0, \pi\}$ and we can also proceed as in the first case.

Thus, given any instance of Equation (K_{old}^*) , its right-hand side can be transformed into

$$\left[\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right] \text{ where}$$

■ $\delta'_1 = \delta_1$

- $\delta'_3 = \delta_3$
- $\delta'_5 = \delta_5$
- $\delta'_7 = \delta_7$
- $\delta'_2 = \begin{cases} \delta_2 & \text{if } \delta_9 \in \{0, \pi\} \\ \delta_9 & \text{if } \delta_9 \in (0, \pi) \\ \delta_9 - \pi & \text{if } \delta_9 \in (\pi, 2\pi) \end{cases}$
- $\delta'_4 = \begin{cases} \delta_4 & \text{if } \delta_9 \in [0, \pi) \\ \delta_4 + 2\pi & \text{if } \delta_9 \in [\pi, 2\pi) \end{cases}$
- $\delta'_6 = \begin{cases} 2\pi - \delta_6 & \text{if } \delta_9 = \pi \text{ and } \delta_6 \neq 0 \\ \delta_6 & \text{else} \end{cases}$
- $\delta'_8 = \begin{cases} \delta_8 + \pi \bmod 2\pi & \text{if } \delta_9 = \pi \text{ and } \delta_6 \neq 0 \\ \delta_8 & \text{else} \end{cases}$.

These angles satisfy the conditions of Figure 2. Indeed, the only case where we can obtain $\delta'_3 = 0$ and $\delta'_2 \neq 0$ in the case distinction above, is the case where $\sin(\frac{2\delta_3}{2}) = 0$, in which $\delta'_6 = \delta_6 = 0$. For the other conditions of Figure 2, the fact that they are satisfied by the δ'_k follows directly from the fact that the δ_j satisfy the conditions of Equation (K_{old}^*) .

The transformation only uses:

- Equations (38), (39), and (42), which are proved in [12] without using Equation (K_{old}^*) and therefore are provable in QC without Equation (K^*) ,
- Lemma 33 and Equations (36) and (37), which only rely on QC without Equation (K^*) ,
- Equation (53), which can be proved using Equation (K_{old}^*) instead of Equation (K^*)
- and Equations (54) and (55), which are consequences of the equations of QC without Equation (K^*) together with Equation (53).

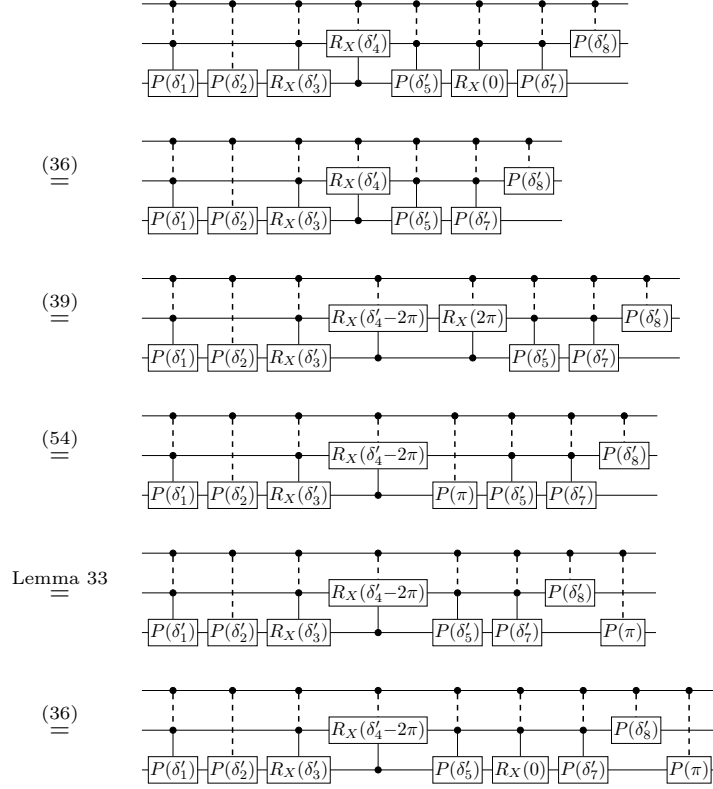
Since Equation (K_{old}^*) has been proved to be sound in [12] (that is, for any angles in its left-hand side, there exist a choice of angles in its right-hand side satisfying the conditions of Equation (K_{old}^*) that makes it sound), and it is easy to see that all equations of QC except maybe Equation (K^*) are sound, this implies that Equation (K^*) is sound.

Moreover, this proves that Equation (K_{old}^*) is a consequence of the equations of QC.

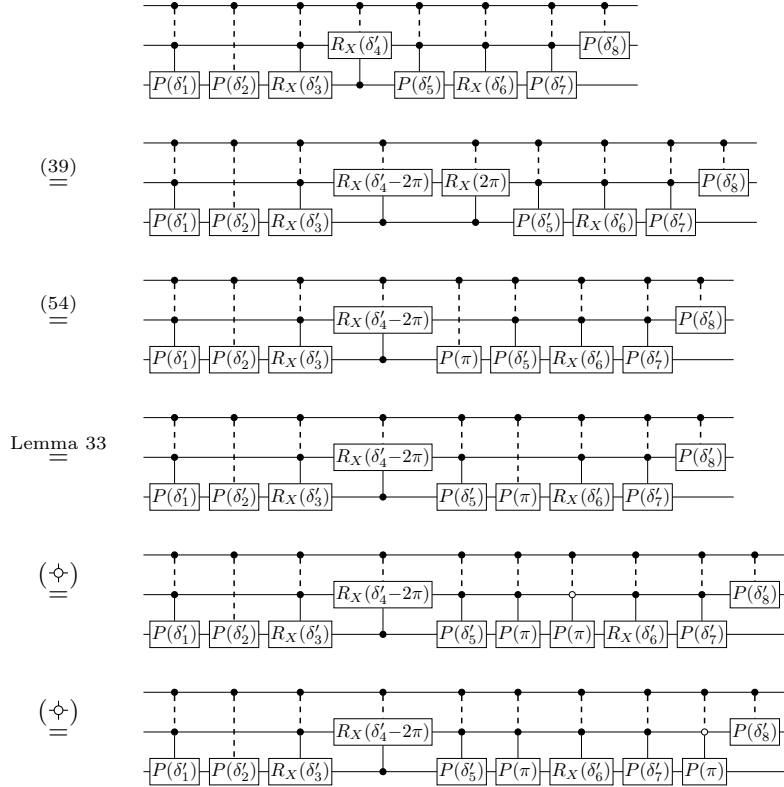
It remains to prove that for any choice of angles in the LHS of Equation (K^*) , the choice of angles in its RHS is unique. To this end, we now consider an instance of Equation (K^*) and transform its RHS into the RHS of the instance of (K_{old}^*) with same LHS. To make easier to differentiate between the parameters of the respective RHS of Equations (K^*) and (K_{old}^*) , we keep denoting those of Equation (K^*) as δ'_k :

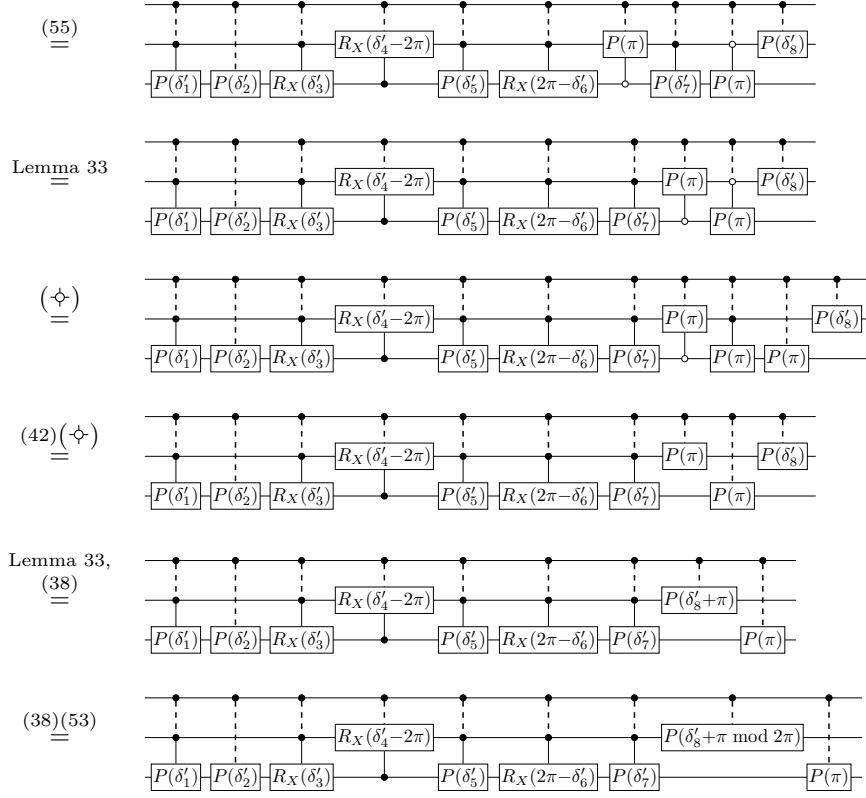
- If $\delta'_4 \in [0, 2\pi)$ and either $\delta'_3 \neq 0$ or $\delta'_2 = 0$, then

- If $\delta'_4 \in [2\pi, 4\pi)$, either $\delta'_3 \neq 0$ or $\delta'_2 = 0$, and $\delta'_6 = 0$, then

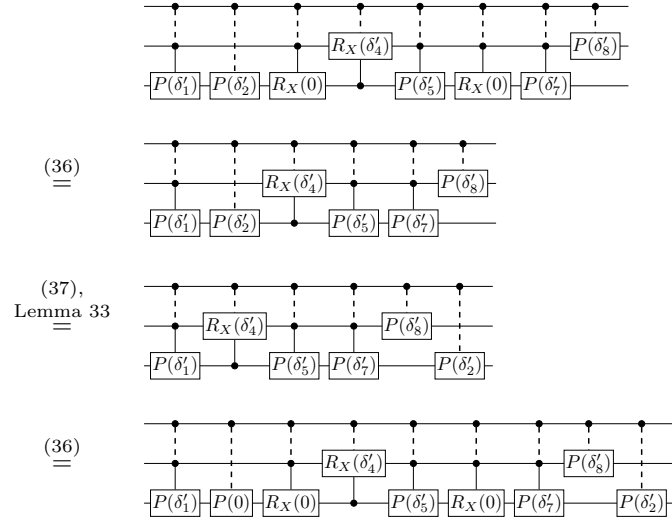


- If $\delta'_4 \in [2\pi, 4\pi)$, either $\delta'_3 \neq 0$ or $\delta'_2 = 0$, and $\delta'_6 \neq 0$, then

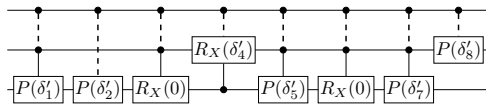




- If $\delta'_4 \in [0, 2\pi)$ but $\delta'_3 = 0$ and $\delta'_2 \neq 0$, then the conditions of Figure 2 imply that $\delta'_6 = 0$, so that



- If $\delta'_4 \in [2\pi, 4\pi)$, $\delta'_3 = 0$ and $\delta'_2 \neq 0$, then the conditions of Figure 2 still imply that $\delta'_6 = 0$, so that



It is easy to check that these angles δ_j satisfy the conditions of Equation (K_{old}^*) whenever the δ'_j satisfy the conditions of Figure 2.

Let g be the function mapping any 8-tuple of angles δ'_k corresponding to the RHS of some instance of Equation (K^*) , to the 9-tuple of angles δ_j given by the formulas just above. Conversely, let f be the function mapping any 9-tuple of angles δ_j corresponding to the right-hand side of some instance of Equation (K_{old}^*) , to the 8-tuple of angles δ'_k given by the formulas given before.

Given any 8-tuple $\vec{\delta}' := (\delta'_k)_{k \in \{1, \dots, 8\}}$ of angles corresponding to the right-hand side of some instance of Equation (K^*) , one has $f(g(\vec{\delta}')) = \vec{\delta}'$. Indeed, let $(\delta_j)_{j \in \{1, \dots, 9\}} := g(\vec{\delta}')$ and $(\delta''_k)_{k \in \{1, \dots, 8\}} := f(g(\vec{\delta}'))$.

- By definition, one has $\delta''_k = \delta'_k$ for $j \in \{1, 3, 5, 7\}$.
- Concerning δ''_2 :
 - If $\delta'_3 \neq 0$ or $\delta'_2 = 0$, then $\delta_2 = \delta'_2$, and δ_9 is either 0 or π depending on δ'_4 , so that $\delta''_2 = \delta_2 = \delta'_2$.
 - If $\delta'_3 = 0$, $\delta'_2 \neq 0$ and $\delta'_4 \in [0, 2\pi)$ then $\delta_9 = \delta'_2 \in (0, \pi)$, so that $\delta''_2 = \delta_9 = \delta'_2$.
 - If $\delta'_3 = 0$, $\delta'_2 \neq 0$ and $\delta'_4 \in [2\pi, 4\pi)$ then $\delta_9 = \delta'_2 + \pi \in (\pi, 2\pi)$, so that $\delta''_2 = \delta_9 - \pi = \delta'_2$.
- Concerning δ''_4 :
 - If $\delta'_4 \in [0, 2\pi)$, then $\delta_4 = \delta'_4$, and δ_9 is either 0 or δ'_2 , which in any case is in $[0, \pi)$, so that $\delta''_4 = \delta_4 = \delta'_4$.
 - If $\delta'_4 \in [2\pi, 4\pi)$, then $\delta_4 = \delta'_4 - 2\pi$, and δ_9 is either π or $\delta'_2 + \pi$, which in any case is in $[\pi, 2\pi)$, so that $\delta''_4 = \delta_4 + 2\pi = \delta'_4$.
- Concerning δ''_6 and δ''_8 :
 - If $\delta'_6 = 0$, then $\delta_8 = \delta'_8$, and $\delta_6 = \delta'_6 = 0$, so that $\delta''_6 = \delta_6 = \delta'_6 (= 0)$ and $\delta''_8 = \delta_8 = \delta'_8$.
 - If $\delta'_4 \in [0, 2\pi)$, then on the one hand, $\delta_6 = \delta'_6$ and $\delta_8 = \delta'_8$, and on the other hand, δ_9 is either 0 or δ'_2 , which in any case cannot be equal to π , so that $\delta''_6 = \delta_6 = \delta'_6$ and $\delta''_8 = \delta_8 = \delta'_8$.
 - If $\delta'_6 \neq 0$ and $\delta'_4 \in [2\pi, 4\pi)$, then the conditions of Figure 2 imply that we cannot have both $\delta'_3 = 0$ and $\delta'_2 \neq 0$, so that $\delta_9 = \pi$, $\delta_6 = 2\pi - \delta'_6$, $\delta''_6 = 2\pi - \delta_6 = \delta'_6$, $\delta_8 = \delta'_8 + \pi \bmod 2\pi$, and since $\delta'_8 \in [0, 2\pi)$, $\delta''_8 = \delta_8 + \pi \bmod 2\pi = \delta'_8$.

Thus, given any instance of Equation (K_{old}^*) , the 8-tuple $\vec{\delta}'$ of the angles of its RHS satisfies $\vec{\delta}' = f(g(\vec{\delta}'))$. Since we have proved that the 9-tuple $g(\vec{\delta}')$ corresponds to the angles of the RHS of the instance of Equation (K_{old}^*) with same LHS, and it has been proved in [12] that this 9-tuple is uniquely determined by the LHS, this proves that the 8-tuple $\vec{\delta}'$ is uniquely determined by the LHS as well.

D Completeness of \mathbf{QC}_{iso}

D.1 Proof of Lemma 15

Proof of Lemma 15. By assumption, C is a $n \rightarrow n + 1$ \mathbf{QC}_{iso} -circuit. The only generator of \mathbf{QC}_{iso} that does not preserve the number of qubits is qubit initialisation \vdash . As there is no generator that reduces the number of qubit, there is exactly one \vdash in the circuit. Using the axioms of prop, we can pull this qubit initialisation to the top left so as to get

$$\begin{array}{c} \vdash \\ \vdots \\ \boxed{C} \\ \vdots \end{array} = \begin{array}{c} \vdash \\ \vdots \\ \boxed{C'} \\ \vdots \end{array} \quad \text{where } C' \text{ is a } \mathbf{QC}\text{-circuit.}$$

Let $U = \llbracket C' \rrbracket$. Since $U(|0\rangle \otimes Id) = |0\rangle \otimes Id$, U is of the form $U = \left(\begin{array}{c|c} I & 0 \\ \hline 0 & U' \end{array} \right)$ with U' unitary. By universality of **QC**-circuits (Proposition 3), there exists a **QC**-circuit $C_{U'}$ that implements U' , using only global phase, phases, Hadamards, CNOTs and swaps. One can

apply the following transformations $\boxed{H} \rightarrow \boxed{P(\frac{\pi}{2})} \boxed{R_X(\frac{\pi}{2})} \boxed{P(\frac{\pi}{2})}$ and $\text{CNOT} \rightarrow \text{CNOT} \text{ with } \oplus \text{ and } \ominus$, it

leads to H -free, swap-free circuit $\tilde{C}_{U'}$ provably equivalent (with **QC**) to $C_{U'}$.

By controlling each of the gates constituting $\tilde{C}_{U'}$ (using definitions in Figure 1, and taking $P(\varphi)$ as the control of global phase φ) with a fresh qubit, we get a circuit $\Lambda \tilde{C}_{U'}$ such that $\llbracket \Lambda \tilde{C}_{U'} \rrbracket = \llbracket C' \rrbracket$, and where the fresh qubit only sees Phases P and the control part of some gates. By completeness of **QC** we have $\text{QC} \vdash C' = \Lambda \tilde{C}_{U'}$ so $\text{QC}_{\text{iso}} \vdash \begin{array}{c} \boxed{C} \\ \vdots \end{array} = \begin{array}{c} \boxed{\Lambda \tilde{C}_{U'}} \\ \vdots \end{array}$.

Thus, one can push the initialisation of $\begin{array}{c} \boxed{\Lambda \tilde{C}_{U'}} \\ \vdots \end{array}$ through all the (controlled) gates using

Equations 49, 50 and 47, leading to $\begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array}$. ◀

D.2 Proof of Lemma 16

To show Lemma 16, we first introduce useful known decompositions, and recall as well the usual (balanced) CSD for reference:

► **Lemma 36** (Matrix Decompositions [47]).

- **RQ (QL):** Let A be a square matrix. There exists Q unitary and R upper triangular (with non-negative diagonal coefficients) such that $A = RQ$. There exists Q' unitary and L lower triangular (with non-negative diagonal coefficients) such that $A = Q'L$.
- **Singular Value (SVD):** For any matrix A , there exist U and V unitary, and $D = \text{diag}(d_1, \dots, d_n)$ real diagonal with $d_i \geq d_{i+1} \geq 0$, such that $A = UDV$.
 $\left(\begin{array}{c|c} I & 0 \\ \hline 0 & U \end{array} \right) \left(\begin{array}{c|c} I & 0 \\ \hline 0 & D \end{array} \right) \left(\begin{array}{c|c} I & 0 \\ \hline 0 & V \end{array} \right)$ is then an SVD of $\left(\begin{array}{c|c} I & 0 \\ \hline 0 & A \end{array} \right)$.
- **(balanced) Cosine-Sine (CSD):** Let $U = \left(\begin{array}{c|c} U_{00} & U_{01} \\ \hline U_{10} & U_{11} \end{array} \right)$ be unitary with U_{ij} all of the same dimension. Then, there exist A_0, A_1, B_0, B_1 unitary, $C = \text{diag}(c_0, \dots, c_n)$ and $S = \text{diag}(s_0, \dots, s_n)$ such that $U = \left(\begin{array}{c|c} A_0 & 0 \\ \hline 0 & A_1 \end{array} \right) \left(\begin{array}{c|c} C & -S \\ \hline S & C \end{array} \right) \left(\begin{array}{c|c} B_0 & 0 \\ \hline 0 & B_1 \end{array} \right)$ and $C^2 + S^2 = I$.

A more general version of the CSD exists for “unbalanced” partitions of U i.e. when the U_{ij} do not not have the same dimensions, but we will not use it in this paper.

Proof of Lemma 16. This is a small variation on the usual CSD. Let us start with $U = \left(\begin{array}{c|c|c} I & 0 & 0 \\ \hline 0 & U_{00} & U_{01} \\ \hline 0 & U_{10} & U_{11} \end{array} \right)$. Let:

- $A_0 C_0 B_0$ be an SVD of U_{00} ,
- $A_1 R$ be a QL decomposition of $\left(\begin{array}{c|c} 0 & U_{10} B_0^\dagger \end{array} \right)$ and

■ LB'_1 be an RQ decomposition of $\begin{pmatrix} 0 \\ A_0^\dagger U_{01} \end{pmatrix}$.

The unitarity forces the diagonal components of C_0 to be between 0 and 1. If 1s appear, they do so as the first diagonal components, as the SVD sorts them from largest to smallest. We then denote C the submatrix of C_0 which has only < 1 components. We

then have: $U = \begin{pmatrix} I & 0 & 0 \\ 0 & A_0 & 0 \\ 0 & 0 & A_1 \end{pmatrix} \begin{pmatrix} I & 0 & R \\ 0 & C & \\ L & A_1^\dagger U_{11} B_1^\dagger & \end{pmatrix} \begin{pmatrix} I & 0 & 0 \\ 0 & B_0 & 0 \\ 0 & 0 & B'_1 \end{pmatrix}$. Notice

that since $C \neq C_0$ in general, A_0 and C may not be of the same dimensions. The orthonormality of the columns (resp. the rows) of the middle matrix forces it to be of the

form: $\begin{pmatrix} I & 0 & 0 & 0 \\ 0 & C & 0 & S' \\ 0 & 0 & X_0 & 0 \\ 0 & S & 0 & C' \end{pmatrix}$ with $C^2 + S^2 = C'^2 + S'^2 = I = C^2 + S'^2 = C'^2 + S^2$. Since

both S and S' are non-negative diagonal, this implies $S = S'$, which then, by unitarity, forces $C' = -C$. Moreover, by unitarity again, X_0 itself is unitary. We hence have

$\begin{pmatrix} I & 0 & 0 & 0 \\ 0 & C & 0 & S' \\ 0 & 0 & X_0 & 0 \\ 0 & S & 0 & C' \end{pmatrix} = \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & C & 0 & -S \\ 0 & 0 & I & 0 \\ 0 & S & 0 & C \end{pmatrix} \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & X_0 & 0 \\ 0 & 0 & 0 & -I \end{pmatrix}$. Wrapping it all up, we

have:

$$U = \begin{pmatrix} I & 0 & 0 \\ 0 & A_0 & 0 \\ 0 & 0 & A_1 \end{pmatrix} \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & C & 0 & -S \\ 0 & 0 & I & 0 \\ 0 & S & 0 & C \end{pmatrix} \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & X_0 & 0 \\ 0 & 0 & 0 & -I \end{pmatrix} \begin{pmatrix} I & 0 & 0 \\ 0 & B_0 & 0 \\ 0 & 0 & B'_1 \end{pmatrix}$$

which gives the desired result with $B_1 := \begin{pmatrix} X_0 & 0 \\ 0 & -I \end{pmatrix} B'_1$. ◀

D.3 Proof of Theorem 17

Proof of Theorem 17. Let C_1 and C_2 be two circuits of $\mathbf{QC}_{\text{iso}}(n, n+k)$, such that $\llbracket C_1 \rrbracket = \llbracket C_2 \rrbracket$. Using the same reasoning as in the proof of Lemma 15, there exist two \mathbf{QC} -circuits

C_{u_1} and C_{u_2} such that $C_i = \begin{array}{c} \text{---} \\ | \\ n: \\ | \\ \text{---} \\ C_{u_i} \\ | \\ k: \\ | \\ \text{---} \end{array}$. By completeness of QC, showing that $C_1 = C_2$ is

equivalent to showing that $\begin{array}{c} \text{---} \\ | \\ n: \\ | \\ \text{---} \\ C_U \\ | \\ k: \\ | \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ | \\ n: \\ | \\ \text{---} \\ \text{---} \\ | \\ k: \\ | \\ \text{---} \end{array}$ for $C_U = C_{u_1} C_{u_2}^\dagger$ (Proposition 6).

Let us denote $U = \llbracket C_U \rrbracket$. Notice that U has to be such that $U \begin{pmatrix} I \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} I \\ 0 \\ \vdots \\ 0 \end{pmatrix}$, which,

by unitarity, means $U = \begin{pmatrix} I & 0 \\ 0 & \star \end{pmatrix}$. Let us now prove that QC_{iso} proves the equality, by reasoning inductively on the number n of initialised qubits.

Case $n = 0$: In that case, there is no initialised qubit, and since $\llbracket U \rrbracket = I$, by completeness of QC, $\text{QC} \vdash U = Id$.

Case $n = 1$: There, we have $U = \begin{pmatrix} I & 0 \\ 0 & U' \end{pmatrix}$. Then Lemma 15 gives directly the expected equality.

Case $n + 1$: U is of the form $U = \begin{pmatrix} I & 0 & 0 \\ 0 & U_{00} & U_{01} \\ 0 & U_{10} & U_{11} \end{pmatrix}$ (with U_{00} and U_{11} square). Notice

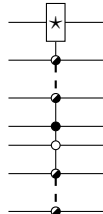
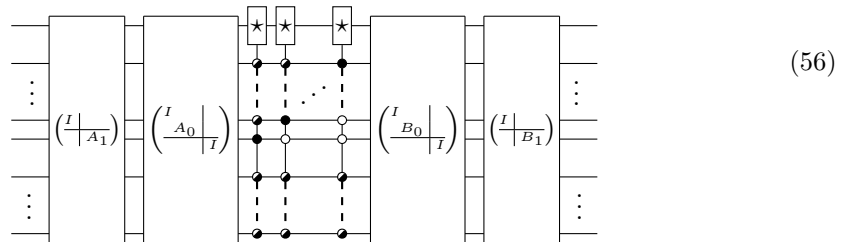
that U has dimension 2^{k+n+1} . We can hence use the modified CSD to get:

$$U = \begin{pmatrix} I & 0 & 0 \\ 0 & A_0 & 0 \\ 0 & 0 & A_1 \end{pmatrix} \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & C & 0 & -S \\ 0 & 0 & I & 0 \\ 0 & S & 0 & C \end{pmatrix} \begin{pmatrix} I & 0 & 0 \\ 0 & B_0 & 0 \\ 0 & 0 & B_1 \end{pmatrix} \text{ with } C^2 + S^2 = I.$$

The middle matrix can be seen as a product of:

$$R_j := c_j |j\rangle\langle j| + s_j |j + 10\dots 0\rangle\langle j| - s_j |j\rangle\langle j + 10\dots 0| + c_j |j + 10\dots 0\rangle\langle j + 10\dots 0| \\ + \sum_{x \notin \{j, j+10\dots 0\}} |x\rangle\langle x|$$

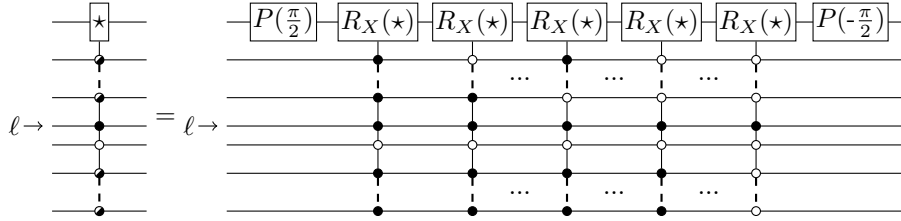
for $\overbrace{0\dots 0}^{n+1} \overbrace{1\dots 1}^k < j < \overbrace{10\dots 0}^{n+k}$ in binary. Notice that the first R_j s might be the identity, if A_0 and C do not have the same dimensions. Notice also that j has at least one 1 in its first $n+1$ bits. R_j is hence a rotation $\begin{pmatrix} c_j & -s_j \\ s_j & c_j \end{pmatrix} = P(\frac{\pi}{2})R_X(\theta_j)P(-\frac{\pi}{2})$ on the first qubit, controlled by all the other qubits. Matrix U can hence be implemented by the following circuit:



where, similarly to [37], e.g. $\ell \rightarrow$ is a syntactic sugar for the composition of all

rotations on the first qubit, controlled by the ℓ -th qubit and anti-controlled by the $\ell + 1$ -th

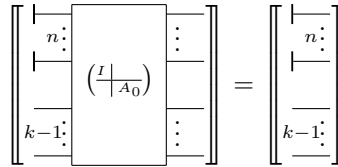
qubit:



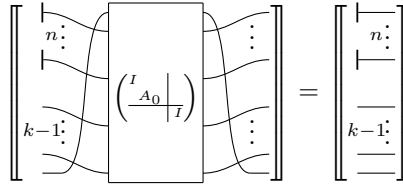
(notice that each R_X should be surrounded by $P(\frac{\pi}{2})$ on the left and $P(-\frac{\pi}{2})$ on the right, but all non-extremal ones simplify using (38) and (D).) By completeness of QC, C_U can be turned into the circuit in (56).

The first block (with A_1) is such that its interpretation satisfies $\forall |\varphi\rangle \in \mathbb{C}^{2^n}, \left(\begin{array}{c|c} I & \\ \hline & A_1 \end{array} \right) (|0\rangle \otimes |\varphi\rangle) = |0\rangle \otimes |\varphi\rangle$, hence using Lemma 15, it is provably deleted by initialisation on the first qubit, and a fortiori when the $n + 1$ first qubits are initialised. Similarly, the last block (with B_1) is deleted by the qubit initialisations.

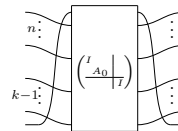
For the second block, notice that:



which implies



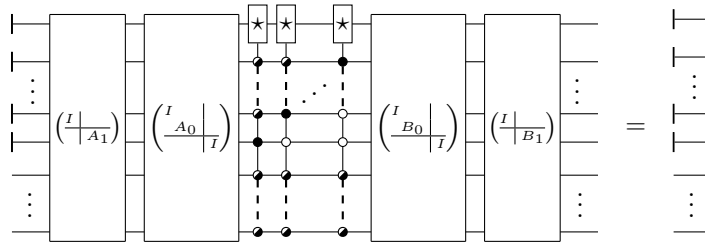
We can hence apply the induction hypothesis on



from which we conclude

that the second block is deleted by initialisations on the $n + 1$ first qubits. Similarly, the penultimate block (with B_0) is deleted by initialisations on the first $n + 1$ qubits.

All the controlled rotations in the middle are deleted by the initialisations thanks to Lemma 15. Finally, it is provable that:



E Completeness of QC_{ancilla}

E.1 Proof of Proposition 21

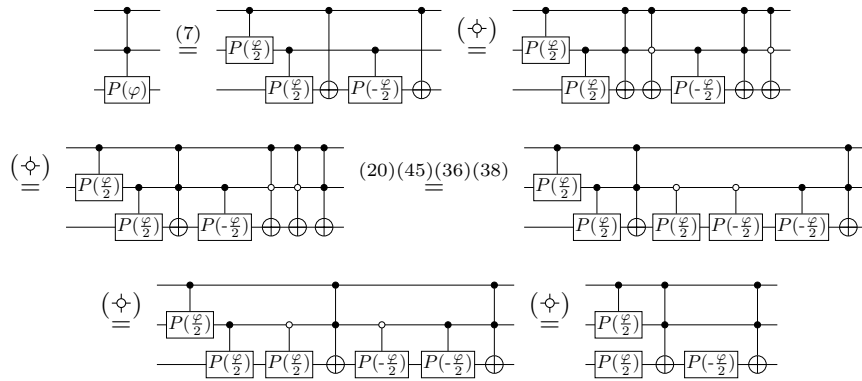
First, we derive the following equations. Equations (57) and (58) are alternative definitions of 2-controlled and 3-controlled phase gates. Equation (59) tells us how we can express a simply controlled gate with Toffoli gates and one 1-qubit gate using one ancilla.

$$\begin{array}{c} \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \text{---} \\ \boxed{P(\varphi)} \end{array} = \begin{array}{c} \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \boxed{P(\frac{\varphi}{2})} \quad \boxed{P(\frac{\varphi}{2})} \\ \oplus \quad \oplus \\ \boxed{P(-\frac{\varphi}{2})} \quad \boxed{P(-\frac{\varphi}{2})} \end{array} \tag{57}$$

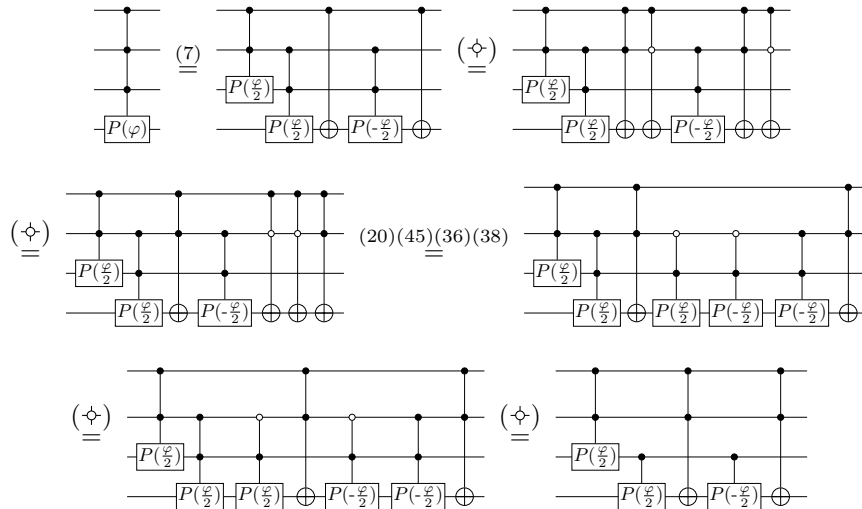
$$\begin{array}{c} \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \text{---} \\ \boxed{P(\varphi)} \end{array} = \begin{array}{c} \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \boxed{P(\frac{\varphi}{2})} \quad \boxed{P(\frac{\varphi}{2})} \\ \oplus \quad \oplus \\ \boxed{P(-\frac{\varphi}{2})} \quad \boxed{P(-\frac{\varphi}{2})} \end{array} \tag{58}$$

$$\begin{array}{c} \bullet \\ \text{---} \\ \text{---} \\ \boxed{P(\varphi)} \\ \text{---} \\ \text{---} \\ \oplus \\ \boxed{P(\varphi)} \end{array} = \begin{array}{c} \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \bullet \\ \text{---} \\ \oplus \\ \boxed{P(\varphi)} \end{array} \tag{59}$$

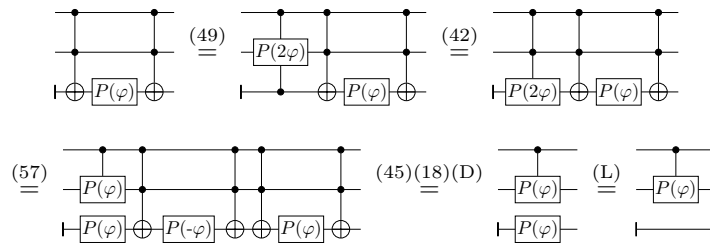
Proof of Equation (57).



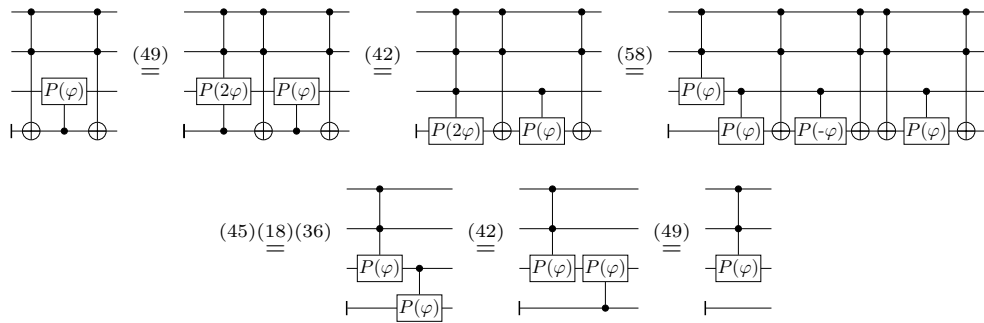
Proof of Equation (58).



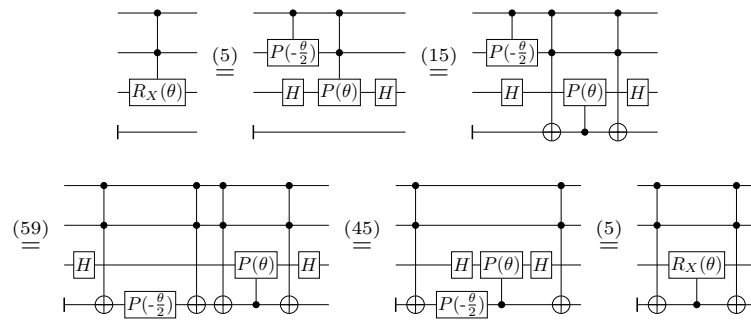
Proof of Equation (59).



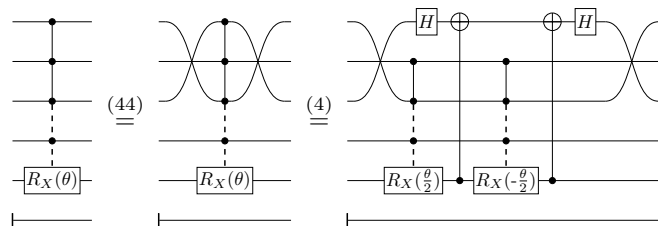
We first prove Equations (15) and (16) by induction on the number of qubits, whose base cases contains $n = 4$ qubits. The base case for Equations (15) can be derived as follows.

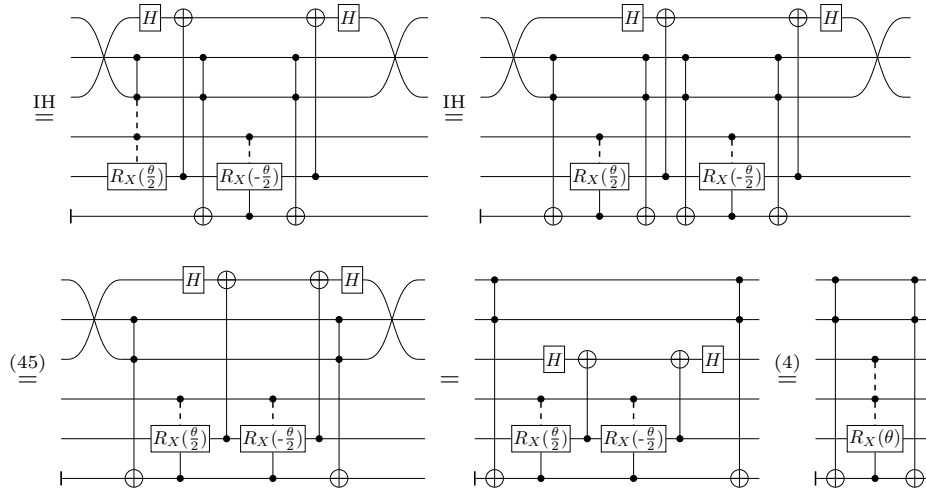


The base case for Equations (15) can be derived as follows.

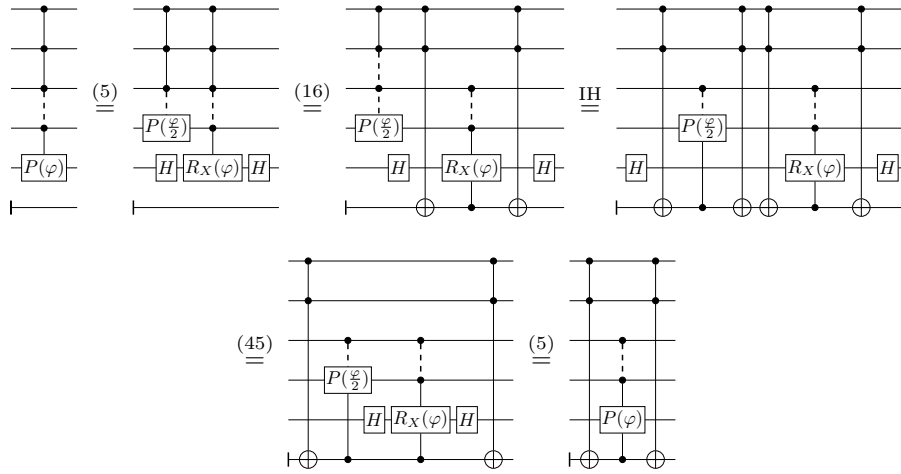


The induction step for Equation (16) can be derived as follows.





The induction step for Equation (15) can be derived as follows.



E.2 Proof of Equation (K^3) in QC_{ancilla}

The main idea of the proof of Equation (K^3) is to use the *Fredkin gate* (or *controlled-swap gate*), defined by Equation (60).

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} := \begin{array}{c} \text{---} \\ \oplus \\ \oplus \\ \oplus \\ \text{---} \end{array} \quad (60)$$

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \quad (K^3)$$

First, we derive some useful equations.

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} = \begin{array}{c} \oplus \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \quad (61)$$

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \quad (62)$$

(63)

(69)

(64)

(70)

(65)

(71)

(66)

(72)

(67)

(73)

(68)

(74)

Proof of Equation (61).

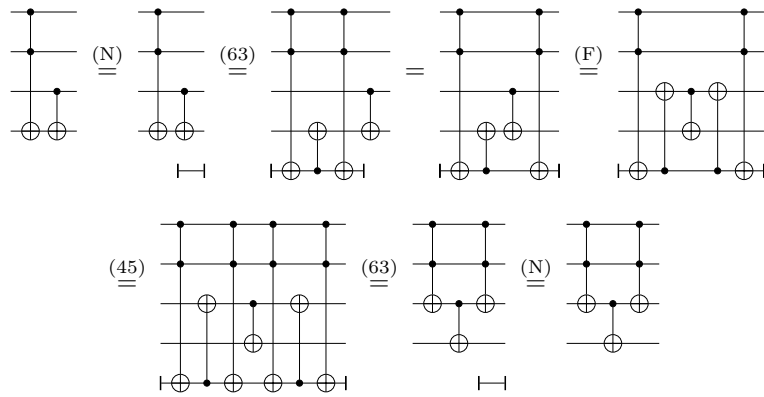


Proof of Equation (62).

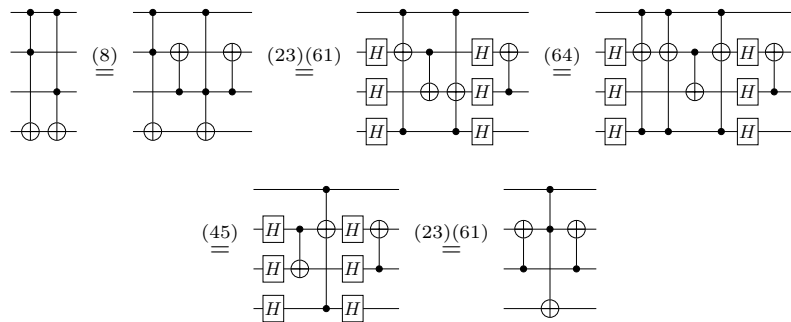


Proof of Equation (63).

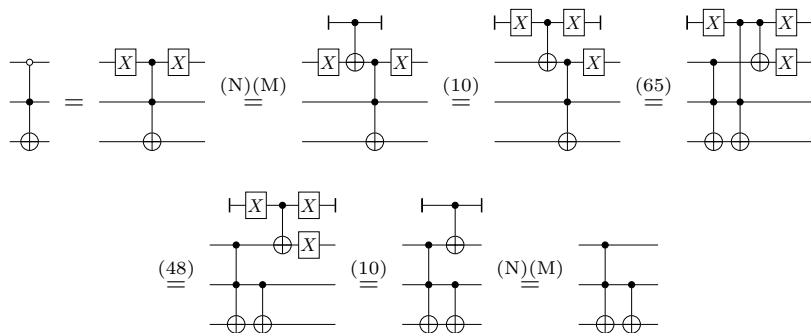
Proof of Equation (64).



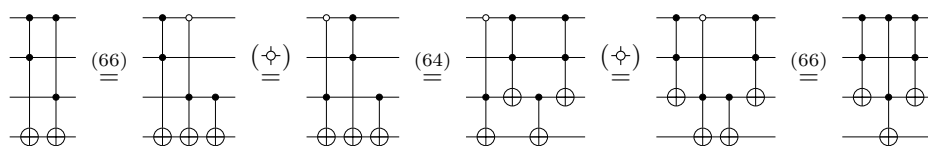
Proof of Equation (65).



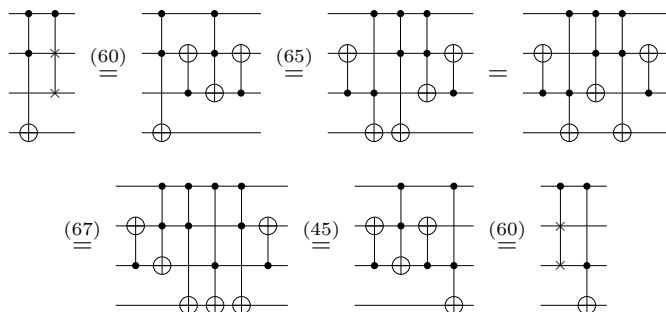
Proof of Equation (66).



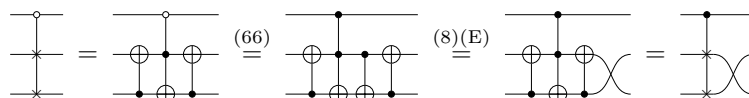
Proof of Equation (67).



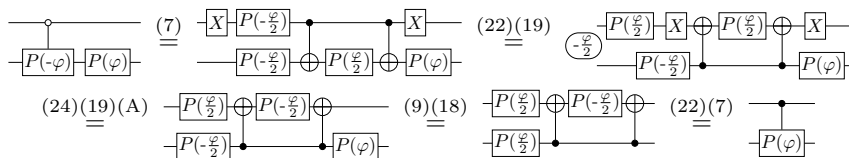
Proof of Equation (68).



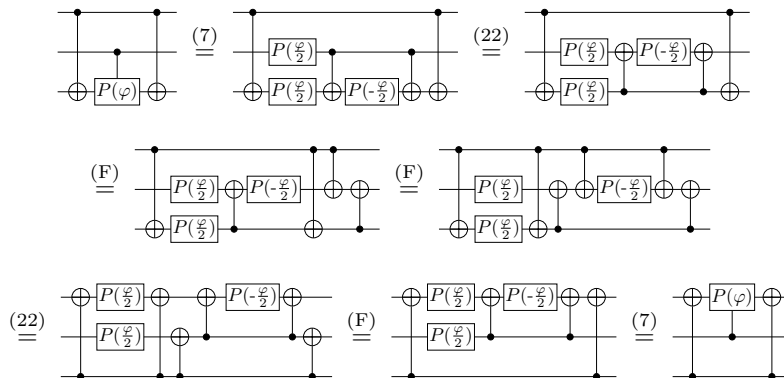
Proof of Equation (69).



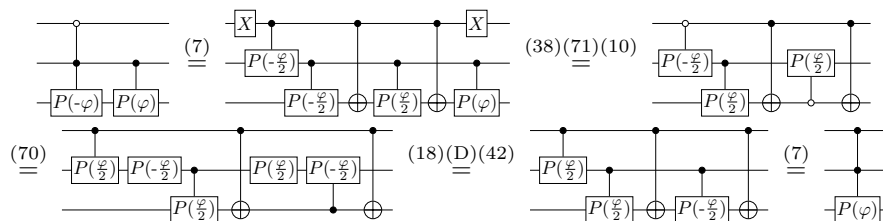
Proof of Equation (70).



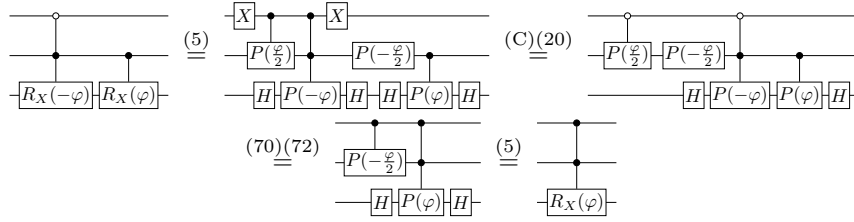
Proof of Equation (71).



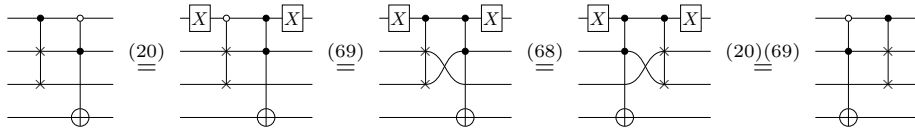
Proof of Equation (72).



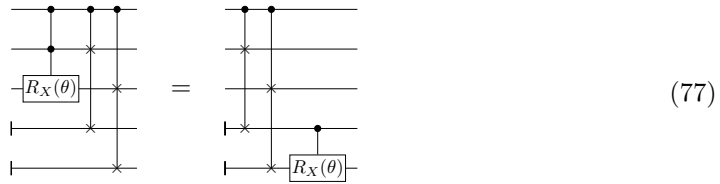
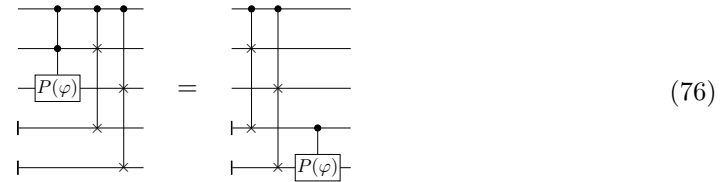
Proof of Equation (73).



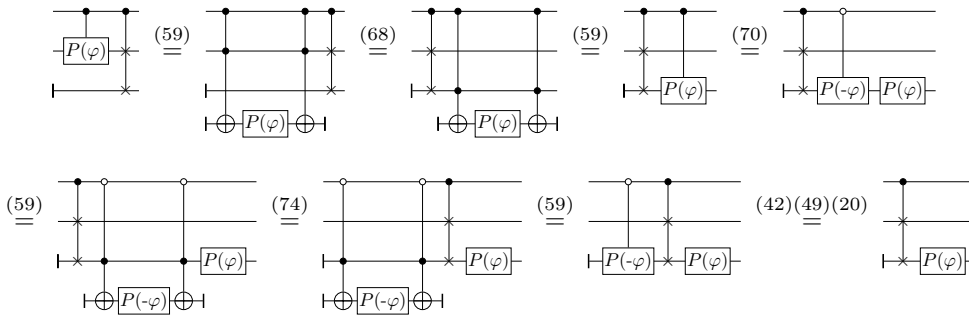
Proof of Equation (74).



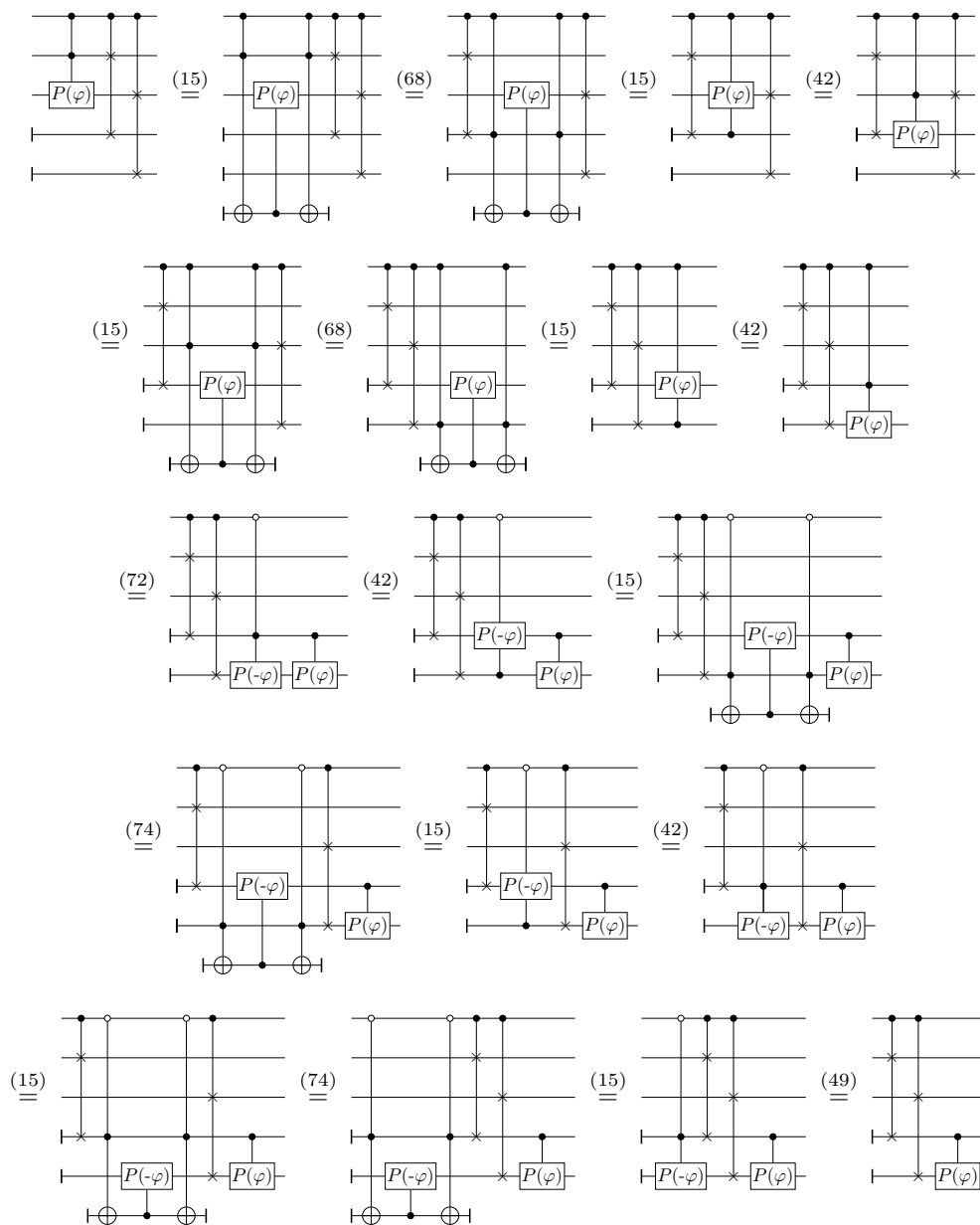
The idea of the proof of Equation (K³) is to start from the LHS circuit of (K³), use Equations (75),(76) and (77) to build an instance of the LHS circuit of (K²) on two ancillae, apply (K²) and then rebuild the RHS circuit of (K³) using the same equations.



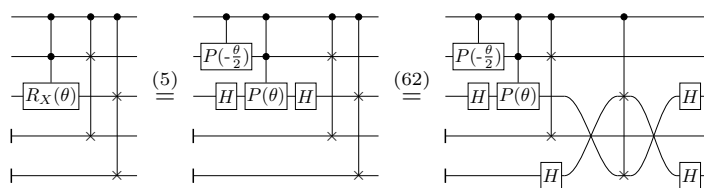
Proof of Equation (75).

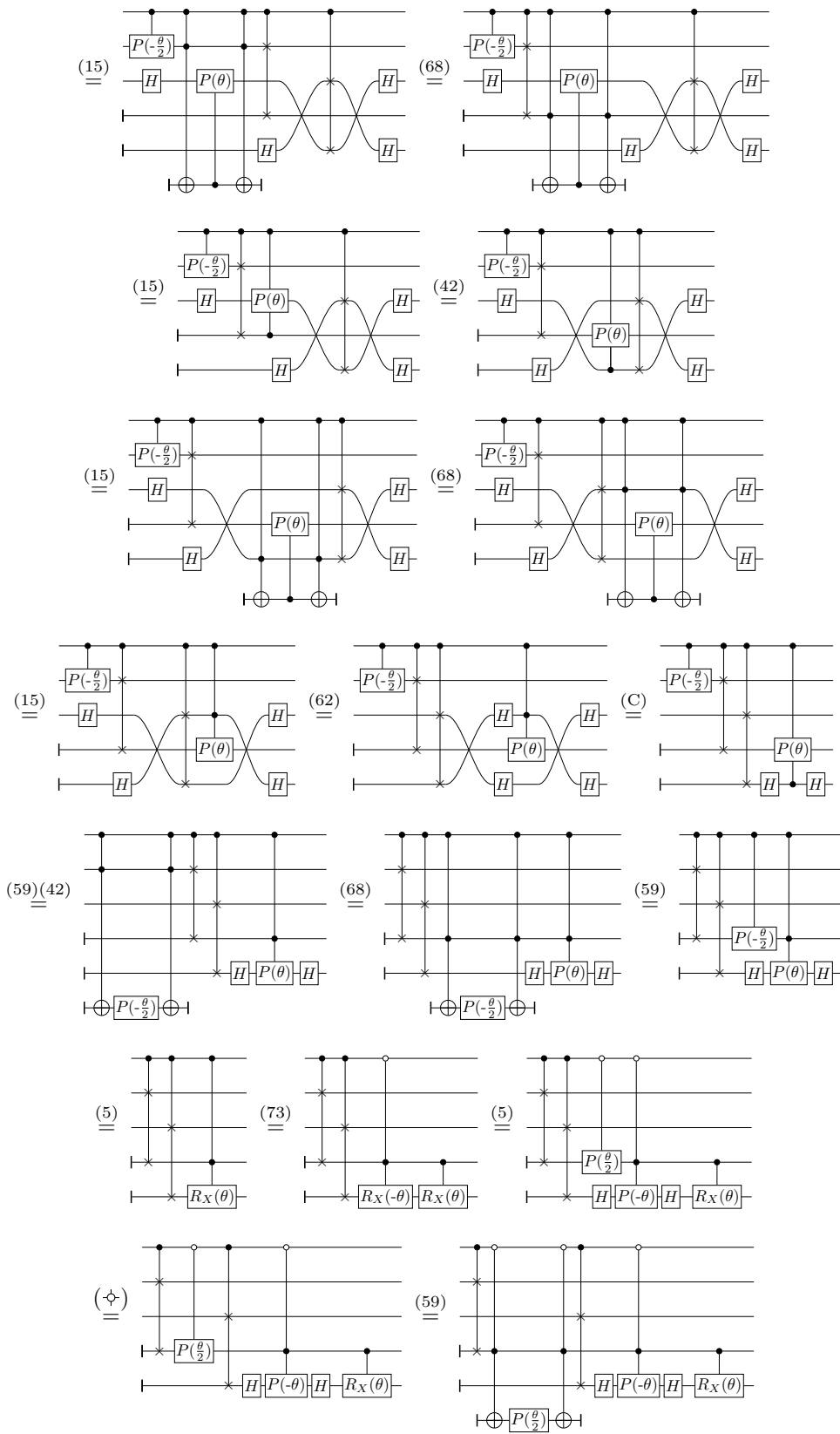


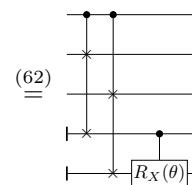
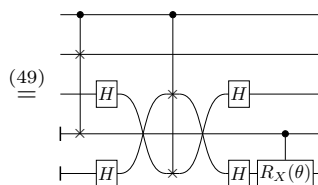
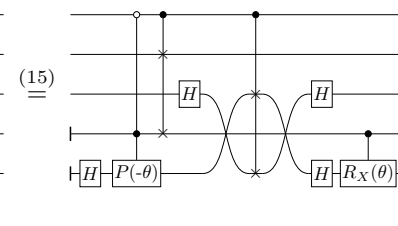
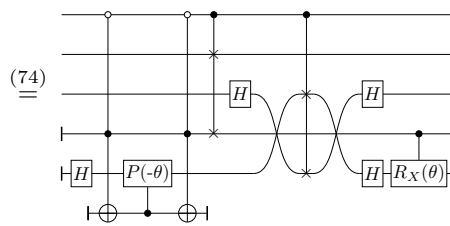
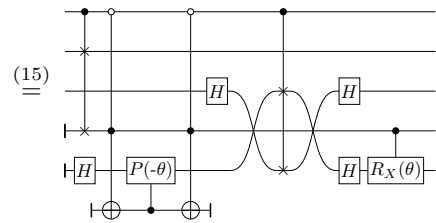
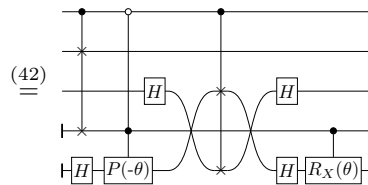
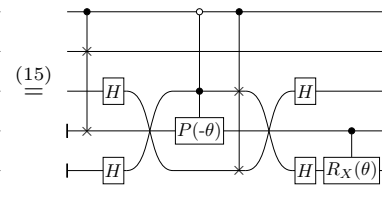
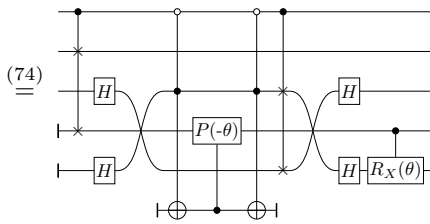
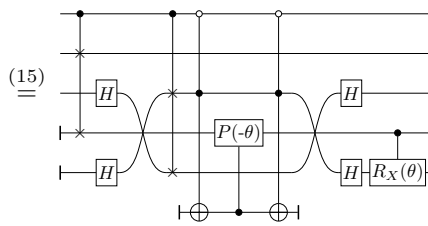
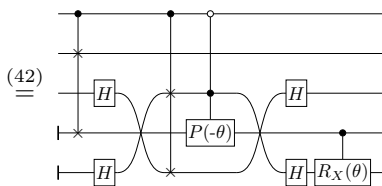
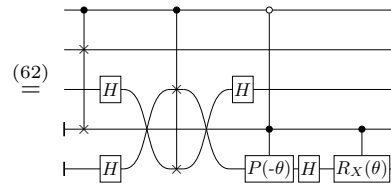
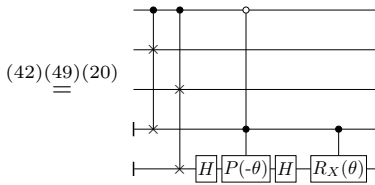
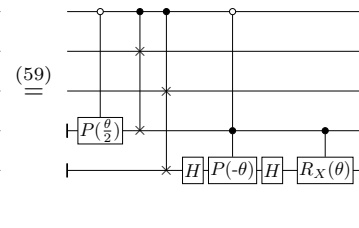
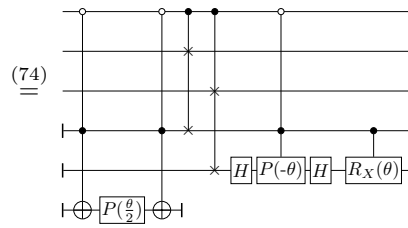
Proof of Equation (76).



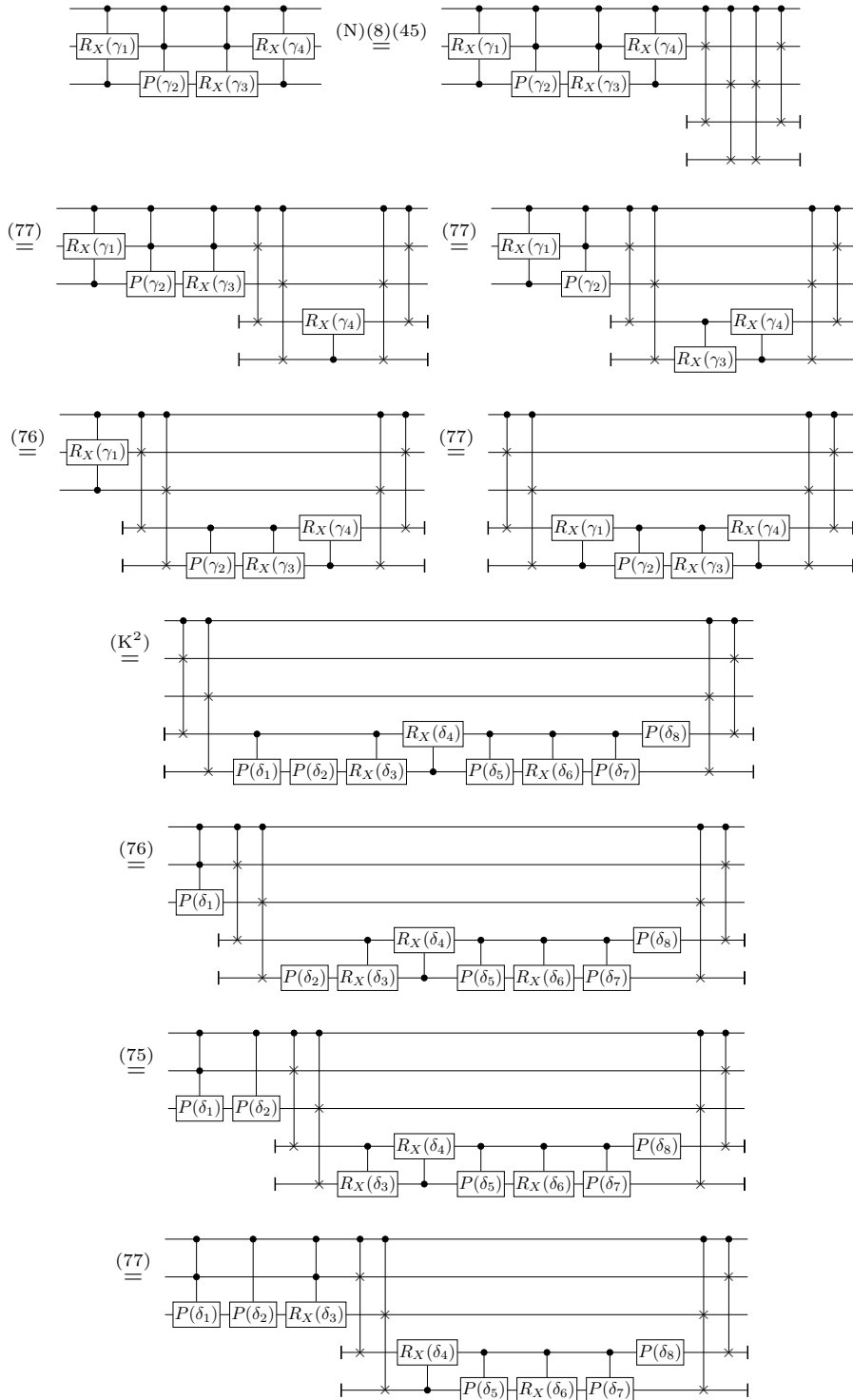
Proof of Equation (77).

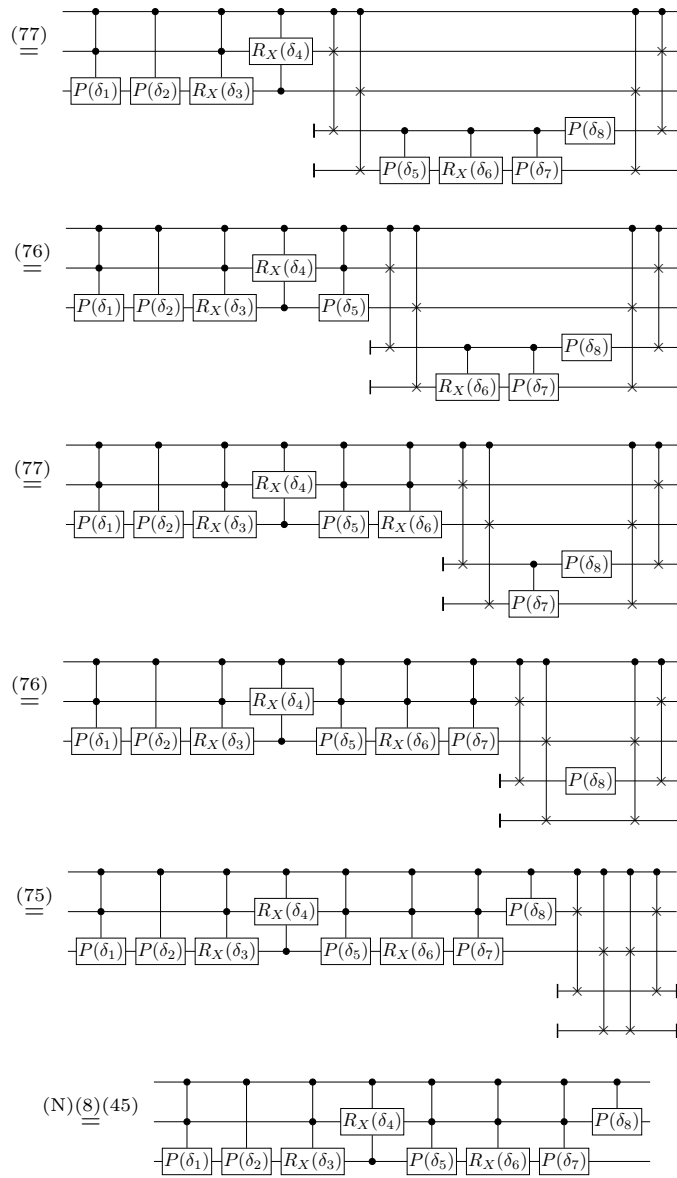






Proof of Equation (K^3) .





E.3 Proof of Equation (K*) in QC_{ancilla}

