

Optimising Clifford Circuits with Quantomatic

Andrew Fagan¹

Ross Duncan^{1,2}

andrew.fagan.2014@uni.strath.ac.uk ross.duncan@strath.ac.uk

¹Department of Computer and Information Sciences
University of Strathclyde
26 Richmond Street, Glasgow, United Kingdom

²Cambridge Quantum Computing Ltd
9a Bridge Street, Cambridge, United Kingdom

We present a system of equations between Clifford circuits, all derivable in the ZX-calculus, and formalised as rewrite rules in the Quantomatic proof assistant. By combining these rules with some non-trivial simplification procedures defined in the Quantomatic tactic language, we demonstrate the use of Quantomatic as a circuit optimisation tool. We prove that the system always reduces Clifford circuits of one or two qubits to their minimal form, and give numerical results demonstrating its performance on larger Clifford circuits.

1 Introduction

Remarkable advances in the past two years have seen quantum computing hardware reach the point where the deployment of quantum devices for non-trivial tasks is now a near-term prospect. However, these machines still suffer from severe limitations, both in terms of memory size and the coherence time of their qubits. It is therefore of paramount importance to extract the most useful work from the fewest operations: a poorly optimised quantum program may not be able to finish before it is undone by noise.

In this paper we study the automated optimisation of *Clifford circuits*. Clifford circuits are not universal for quantum computation – they are well known to be efficiently simulable by a classical computer [2] – however adding any non-Clifford gate to the Cliffords yields a set of approximately universal operations hence it is likely that the vast majority of operations in any quantum program will be Clifford operations, and hence reducing the Clifford depth and gate count of a circuit will have substantial benefit.

A secondary reason to focus on Cliffords is that the corresponding subtheory of quantum mechanics is well-understood in terms of the ZX-calculus [7]. Backens [3] has shown that the ZX-calculus is sound and complete for *stabilizer quantum theory* – that is the fragment of quantum mechanics containing only the Clifford operations and states which can be produced from them. While recent extensions to the ZX-calculus have been proposed which are complete for the Clifford+T fragment [16] and for the full qubit theory [22], both these extensions are significantly larger and more complex than the stabilizer subtheory, and both axiomatisations are undergoing rapid development. Clifford circuits therefore provide a stable platform to develop techniques which could later be extended to a universal language.

In this work we present a *circuit optimiser* which can transform a Clifford circuit into an equivalent circuit with reduced depth and total number of operations. The system always reduces Clifford circuits of one or two qubits to their minimal form, and yields significant size reductions for larger circuits.

The optimiser has been developed as a *simplification procedure* in the graphical proof-assistant Quantomatic [17, 18]. By working inside the proof-assistant we obtain an important benefit: alongside the optimised circuit our optimiser produces a formal proof certifying the correctness of its circuit transformations.

Quantomatic is a flexible graph rewrite engine which is especially well-adapted to working with the ZX-calculus. It is designed for interactive use, and a typical session involves interleaving automated tactics¹, backtracking, and manually choosing rewrites. However, our circuit optimiser is designed to operate without user intervention, and we have necessarily made extensive use of the Quantomatic’s powerful tactic combinators and its built-in Python interpreter. In doing so, we have constructed the largest and most sophisticated Quantomatic development to date.

As a graph rewriting engine, Quantomatic normally inspects only the local subgraph structure of a term while searching for a rewrite to apply. However, quantum circuits have a global causal structure which must be maintained to preserve the property of “being a circuit”. A key contribution of this work is the development of techniques to infer the global structure and use it to guide the rewrite process.

Selinger [25] presented generators and relations for all the n -qubit Clifford groups as a rewrite system over string diagrams. This work has some similarities to that: most notably, we also treat Clifford circuits as a free PROP subject to an equivalence relation defined on small subgraphs. However Selinger’s approach is based on transforming circuits to a standard form which is often larger than the smallest equivalent circuit, whereas we aim for minimal forms. Selinger’s rewrite system has a much larger number of rules than the axioms of the ZX-calculus. Maslov and Roetteler [21] demonstrate that all Clifford unitaries can be implemented in depth no more than 7 stages deep, using the $\wedge Z$ as the only two-qubit gate. The $\wedge Z$ has formal disadvantages in ZX-calculus, so in our development we have used the CNOT and swap gates instead. In the examples we have tested, our optimiser usually attains similar depth over our gate set; however on some examples it halts while some simplifications are still possible. Quantomatic has previously been used to produce mechanised correctness proofs for quantum error correcting codes [14, 6, 11], and many of the techniques used in these works are applied here.

We assume that the reader is at least somewhat familiar with both the ZX-calculus and the Quantomatic system; an accessible introduction to both is found in the earlier formalisation effort [14].

Acknowledgements The authors wish to thank Aleks Kissinger and Hector Miller-Bakewell for their technical assistance throughout this project.

The Quantomatic project files All the proofs which appear in this paper and its appendix are publicly available as a downloadable Quantomatic project at <https://gitlab.cis.strath.ac.uk/kwb13215/Clifford-Quanto/>.

2 The Clifford Group

Let $\omega = e^{i\pi/4}$. The n th Clifford group is the group of unitary matrices acting on \mathbb{C}^{2^n} , finitely generated by the matrices

$$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \quad V = \frac{1}{\sqrt{2}} \begin{pmatrix} \omega & \bar{\omega} \\ \bar{\omega} & \omega \end{pmatrix} \quad \text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad \sigma = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

under tensor product and matrix composition. Observe that S and V are both order 4, the Pauli matrices are given by $Z = S^2$ and $X = V^2$, and the usual Hadamard matrix is obtained as $H = \bar{\omega}SVS$. Throughout

¹A *tactic* is a short program which automates a particular proof strategy.

this paper we will quotient the group by global scalar factors, so that $A = zA$ for all non-zero $z \in \mathbb{C}$. The resulting quotient yields the n th *reduced* Clifford group, which we denote \mathcal{C}_n .

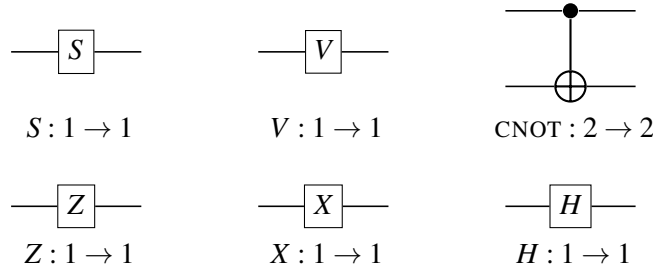
\mathcal{C}_n is finite for all n and the order of the group is given by the expression²:

$$|\mathcal{C}_n| = \prod_{j=1}^n 2(4^j - 1)4^j = 2^{2n+1}(2^{2n} - 1)|\mathcal{C}_{n-1}|.$$

The order of \mathcal{C}_n grows very quickly: $|\mathcal{C}_1| = 24$, $|\mathcal{C}_2| = 11520$, $|\mathcal{C}_3| = 92827280$, and so on.

The Clifford group [15] is equivalently defined as the *normalizer* of the Pauli group within the unitaries. Let \mathcal{P}_n be the subgroup of \mathcal{C}_n generated by the Z and X operators³. Then for all $C \in \mathcal{C}_n$ and all $P \in \mathcal{P}_n$ we have $CP = P'C$ for some $P' \in \mathcal{P}_n$. This crucial fact will heavily exploited in our circuit optimisation procedure.

A more holistic view of the Cliffords is as a class of *circuit diagrams* whose gates are the generators of the group, rather than the group itself. This can be formalised as a free \dagger -PROP [20, 19] generated by morphisms



We refer to this PROP as **Cliff**. Note that the swap σ is automatically present due to the PROP structure. The morphisms Z , X , and H are not essential, but it will be convenient later to include them among the generators. The matrix valuations above suffice to define a standard interpretation functor $[\![\cdot]\!]_C : \mathbf{Cliff} \rightarrow \mathbf{fdHilb}$, such that $[\![\mathbf{Cliff}(n, n)]\!]_C = \mathcal{C}_n$. We will use this PROP only to define the translation from **Cliff** to the ZX-calculus as a functor; we refer the interested reader to Selinger [25] for more details of this perspective.

Remark 2.1. Note that **Cliff**, as a free PROP, does not include any non-trivial equations between Clifford circuits and is not therefore a presentation of the Clifford *group* itself: **Cliff** distinguishes between different implementations of the same unitary map, which are identified in the image of $[\![\cdot]\!]_C$. In particular $\mathbf{Cliff}(n, n)$ is infinite for all $n > 0$.

Remark 2.2. Although it will play only a minor role in this paper, we stress that **fdHilb** denotes the category of finite dimensional Hilbert spaces and linear maps under the quotient described above: $A = zA$ for all non-zero $z \in \mathbb{C}$. It is common to impose this quotient only for $z = e^{i\alpha}$, however in this work the question of normalisation will not arise.

3 The ZX-calculus

The ZX-calculus [7] is a formal graphical notation for representing quantum states and processes, and an equational theory for reasoning about them. It is *universal*, meaning that every linear map has a

²The only scalars which arise in the quotient are ω^k for $k \in \mathbb{N}$ so the usual Clifford group is eight times larger.

³Under our quotient we have $Y = ZX = XZ$ so these generators suffice.

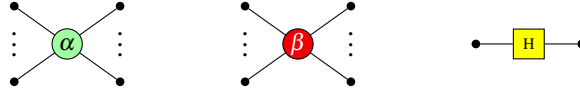


Figure 1: Allowed interior vertices

corresponding ZX-calculus term, and *sound*, meaning that any equation derivable in the calculus is true in its standard Hilbert space interpretation.

The ZX-calculus is formalised using *open graphs*, a generalisation of the usual notion of graph. Open graphs have three kinds of edges: *closed* edges have a vertex at each end, as in a conventional graph; *half-open* edges are incident upon a single vertex, the other end being open; and *open* edges are open at both ends, being incident upon no vertices. The set of open ends of the edges form the *boundary* of the open graph. An open graph is called *framed* if additionally the boundary is partitioned into two linearly ordered sets of *inputs* and *outputs*.

Definition 3.1. A *term*, or *diagram*, of the ZX-calculus is a finite undirected framed open graph whose interior vertices are of the following types:

- $Z(\alpha)$ vertices, labelled by an angle α where $0 \leq \alpha < 2\pi$. These are depicted as green or light grey circles; if $\alpha = 0$ then the label is omitted.
- $X(\beta)$ vertices, labelled by an angle β , where $0 \leq \beta < 2\pi$. These are depicted as red or dark grey circles; again, if $\beta = 0$ then the label is omitted.
- H vertices; unlike the other types H vertices are constrained to have degree exactly 2. They are depicted as yellow squares.

Two terms are considered equal if they are isomorphic as framed labelled graphs.

The allowed vertex types are shown in Figure 1. We adopt the convention that inputs are on the left, and outputs on the right.

Compound terms may be formed by joining some number (maybe zero) of the outputs of one term to the inputs of another. Given a diagram $D : n \rightarrow m$ we define its *adjoint* $D^\dagger : m \rightarrow n$ to be the diagram obtained by reflecting the diagram around the vertical axis and negating all the angles. Thus the terms of the ZX-calculus naturally form a \dagger -PROP [8, 10], just like the Clifford circuits of the previous section. The three types of single vertex shown in Figure 1 can then be seen as the generators of this PROP, which we call **ZX**.

Remark 3.2. We consider the *scalar-free* fragment of the ZX-calculus; or equivalently, we quotient everything by non-zero scalar factors, just as we did in the previous section. This greatly reduces the complexity of the diagrams and poses no danger; Backens has demonstrated how to modify the calculus to preserve equality while respecting scalars [4].

Definition 3.3. Given a zx-term $D : m \rightarrow n$, its *standard interpretation* is a linear map $\llbracket D \rrbracket : (\mathbb{C}^2)^{\otimes m} \rightarrow (\mathbb{C}^2)^{\otimes n}$ defined on single vertices as follows:

$$\begin{aligned} \left[\begin{array}{c} \bullet \\ \vdots \\ \bullet \end{array} \begin{array}{c} \alpha \\ \bullet \\ \vdots \\ \bullet \end{array} \begin{array}{c} \bullet \\ \vdots \\ \bullet \end{array} \right] &= \left\{ \begin{array}{l} |0\rangle^{\otimes m} \mapsto |0\rangle^{\otimes n} \\ |1\rangle^{\otimes m} \mapsto e^{i\alpha} |1\rangle^{\otimes n} \end{array} \right. & \left[\begin{array}{c} \bullet \\ \vdots \\ \bullet \end{array} \begin{array}{c} \beta \\ \bullet \\ \vdots \\ \bullet \end{array} \begin{array}{c} \bullet \\ \vdots \\ \bullet \end{array} \right] &= \left\{ \begin{array}{l} |+\rangle^{\otimes m} \mapsto |+\rangle^{\otimes n} \\ |-\rangle^{\otimes m} \mapsto e^{i\beta} |-\rangle^{\otimes n} \end{array} \right. \end{aligned}$$

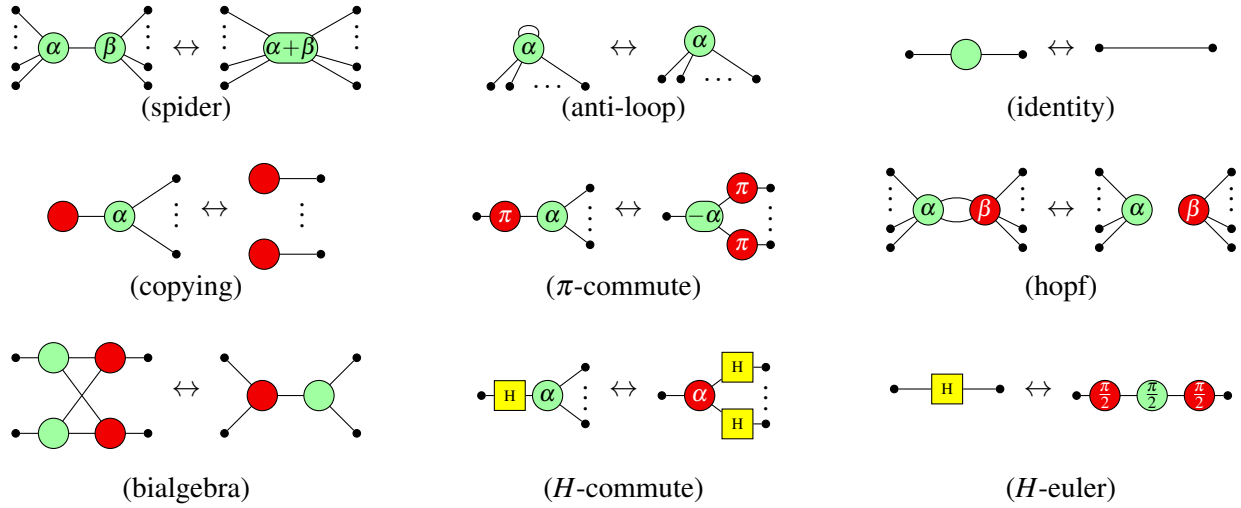


Figure 2: The rules of the ZX-calculus. Note all arithmetic is modulo 2π .

$$\llbracket \bullet \text{---} \boxed{H} \text{---} \bullet \rrbracket = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Since the above diagrams are the generators of \mathbf{ZX} , the above definition extends uniquely to a strict \dagger -symmetric monoidal functor $\llbracket \cdot \rrbracket : \mathbf{ZX} \rightarrow \mathbf{fdHilb}$.

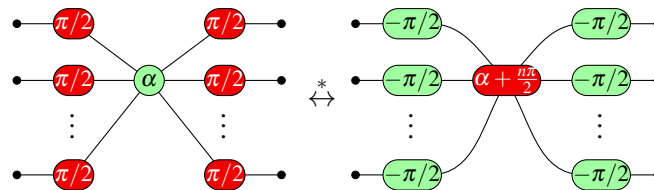
The ZX-calculus has a rich equational theory based on the theory of Frobenius-Hopf algebras [7, 10]. Various axiomatisations have been proposed ([12, 13, 5, 23, 16, 22]) with various advantages and drawbacks. Here we adopt the scheme of Backens [3] which is clean, concise, and adequate for the treatment of the Clifford group. These are shown in Figure 2. Note that, due to the H -commute rule, the colour swapped versions of all the rules are admissible, and we shall use these colour swapped versions without further comment.

Definition 3.4. Let \leftrightarrow be the one-step rewrite relation on the terms of \mathbf{ZX} generated by the pairs of terms shown in Figure 2; let $\overset{*}{\leftrightarrow}$ be the least equivalence relation containing \leftrightarrow . We say that \mathbf{ZX} terms a and b are *equivalent* when $a \overset{*}{\leftrightarrow} b$.

We reserve the notation $a = b$ for the case where a and b are equal as graphs, in the sense of Definition 3.1.

Thanks to the H -euler rule, the H vertices are redundant. With this in mind, the following colour changing rule will be useful.

Lemma 3.5. *The following rule is admissible:*



where n is the number of red vertices in the left hand side diagram.

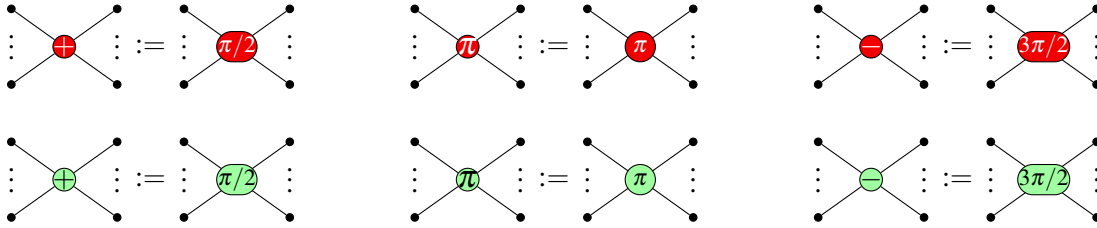
The proof is given in Appendix C.

4 Representing Clifford Circuits in the ZX-calculus

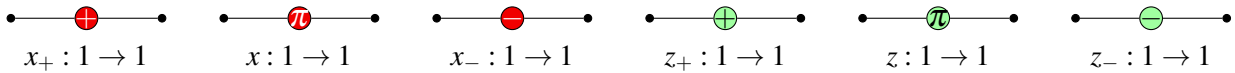
For the rest of the paper we will use only the *stabilizer* sub-language of the full ZX-calculus.

Definition 4.1. Let \mathbf{ZX}_s denote the sub-PROP of \mathbf{ZX} obtained by restricting to those terms whose Z and X vertices are labelled only by angles $\alpha \in \{0, \pi/2, \pi, 3\pi/2\}$.

Since only four vertex labels can occur in the terms of \mathbf{ZX}_s , we will adopt a more compact notation as shown in below.

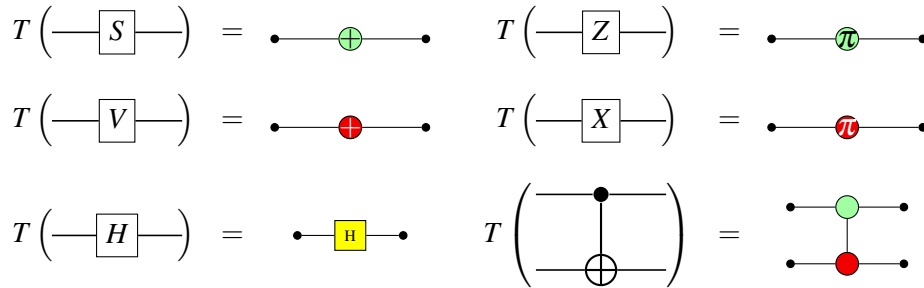


Since the one-qubit instances of these will occur very frequently in the rest of the paper, we introduce the names:



We refer to x and z as the *Paulis*.

We define the *translation functor* $T : \mathbf{Cliff} \rightarrow \mathbf{ZX}_s$ on the generators as shown below.



This extends to the whole PROP in the usual way. Further we have the following:

Proposition 4.2. For all $c : n \rightarrow m$ in \mathbf{Cliff} we have $\llbracket c \rrbracket_C = \llbracket T(c) \rrbracket$.

Subject to the proviso that the variables α and β occurring in the rules of Figure 2 must take values in the set $\{0, \pi/2, \pi, 3\pi/2\}$, it is immediate that if $a \stackrel{*}{\leftrightarrow} b$ then a is in \mathbf{ZX}_s if and only if b is. Further, the equational theory of \mathbf{ZX}_s is sound and complete for its standard interpretation.

Theorem 4.3 (Backens [3]). Let a and b be terms of \mathbf{ZX}_s . Then $a \stackrel{*}{\leftrightarrow} b$ if and only if $\llbracket a \rrbracket = \llbracket b \rrbracket$.

This theorem guarantees that if a given Clifford circuit has a smaller equivalent circuit then there is a proof of their equivalence in the ZX-calculus. The challenge is to find it. We start by considering minimal forms for \mathcal{C}_1 and \mathcal{C}_2 .

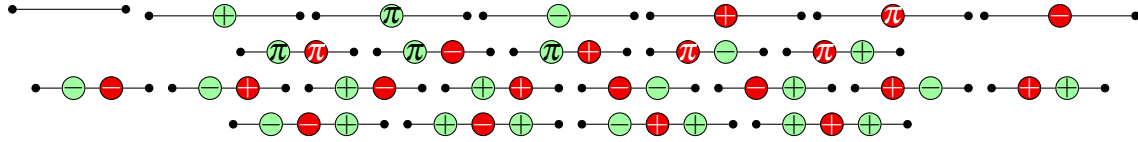


Figure 3: \mathcal{C}_1 : standard minimal forms for single-qubit Cliffords

4.1 1-Qubit Cliffords

Let \mathcal{C}_1 denote the 24 diagrams shown Figure 3. Note that all of them are in the image of the translation functor T , so they correspond to Clifford circuits. Further, each of the diagrams has a distinct interpretation under $\llbracket \cdot \rrbracket$, so they cover \mathcal{C}_1 and, by soundness, they are not equivalent.

Proposition 4.4. *Given $t \in \mathbf{Cliff}(1, 1)$ then $T(t) \overset{*}{\leftrightarrow} c$ for some $c \in \mathcal{C}_1$.*

Proof. From its type, we have $\llbracket t \rrbracket_C \in \mathcal{C}_1$ and since $|\mathcal{C}_1| = 24$, necessarily $\llbracket t \rrbracket_C = \llbracket c \rrbracket$ for some $c \in \mathcal{C}_1$, and thus by Proposition 4.2 $\llbracket T(t) \rrbracket = \llbracket c \rrbracket$. From this point the result follows by Theorem 4.3. \square

Since we will require an effective procedure later, we offer an alternative, constructive, proof which produces the required c . The ideas of this proof form an important part of our optimisation procedure.

Recall that a *line graph* is a framed open graph with one input and one output, which is connected and whose vertices all have degree two. In other words, the graph has the shape of a line. We can treat a line graph as a sequence of vertices starting from the input; let $\text{pos}(v)$ denote the sequence position of vertex v , i.e. if v is the first vertex then $\text{pos}(v) = 0$.

Lemma 4.5. *Let $t \in \mathbf{ZX}_s(1, 1)$ be a line graph; then $t \overset{*}{\leftrightarrow} s$ for some $s \in \mathbf{ZX}_s(1, 1)$ which has the following properties:*

- its vertices form an alternating sequence of $Z(\alpha)$ and $X(\beta)$ vertices, where none of the labels are zero;
- it contains at most two Pauli vertices, and if present these are first vertices after the input.

We say that s is in Pauli-standard form.

Proof. Observe that by applying the H -euler rule all the H vertices can be removed. Then, by repeated application of the spider and identity rules, we obtain a graph of alternating coloured vertices, none of which are labelled by zero. Now we proceed by induction; define

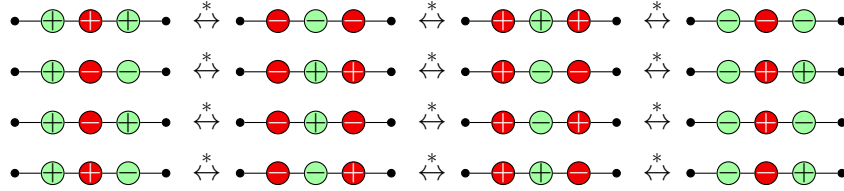
$$m(t) = \sum_{v \text{ is a Pauli}} \text{pos}(v)$$

Observe that if $m(t) < 2$ then t has the required form. Otherwise there is at least one Pauli vertex v with $\text{pos}(v) \geq 2$. Suppose that v is a Pauli Z vertex; then we may rewrite $t \overset{*}{\leftrightarrow} t'$ by the following rewrites:

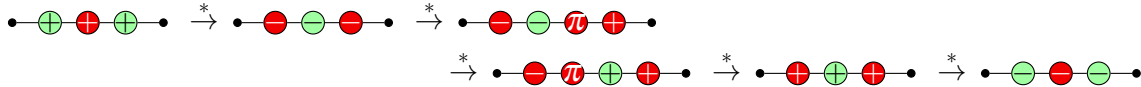
$$\bullet \text{---} \overset{\circlearrowleft}{\alpha} \text{---} \overset{\circlearrowright}{\beta} \text{---} \overset{\circlearrowleft}{\pi} \text{---} \overset{\circlearrowright}{\gamma} \text{---} \bullet \xrightarrow{*} \bullet \text{---} \overset{\circlearrowleft}{\alpha} \text{---} \overset{\circlearrowleft}{\pi} \text{---} \overset{\circlearrowright}{-\beta} \text{---} \overset{\circlearrowright}{\gamma} \text{---} \bullet \xrightarrow{*} \bullet \text{---} \overset{\circlearrowleft}{\alpha + \pi} \text{---} \overset{\circlearrowright}{\gamma - \beta} \text{---} \bullet$$

and applying the identity rule if possible. Note that $Z(\alpha + \pi)$ is never a Pauli, so the number of Paulis is not increased, and the number vertices overall is reduced. If $X(\gamma - \beta)$ is a Pauli then its position is $\text{pos}(v) - 1$. Hence $m(t') < m(t)$, and result is achieved by induction. If v is a Pauli X vertex, then the same argument goes through with the colours reversed. \square

Lemma 4.6. *We have the following equations:*



Proof. For the first sequence of equations, consider the following rewrites



where the first and last steps use Lemma 3.5. The other three cases are established using very similar reasoning. \square

Alternative proof of Prop 4.4. First observe that for any $t \in \mathbf{Cliff}(1, 1)$ its image $T(t)$ has the form of a line graph. Now, by Lemma 4.5, $T(t) \xleftrightarrow{*} t_1$ where t_1 is in Pauli-standard form. Now we proceed by induction on n , the number of vertices of t_1 .

If $n = 0$ or 1 then t_1 is already in \mathcal{C}_1 . If $n = 2$ and t_1 has no Pauli nodes, then t_1 is already in \mathcal{C}_1 ; otherwise $t_1 \xleftrightarrow{*} c$ for some c in \mathcal{C}_1 by the π -commute rule.

If $n = 3$ and t_1 contains at least one Pauli vertex, then by applying the π commute and spider rules, t_1 can rewrite to a term with only two vertices or fewer. For example

$$\bullet \text{---} \pi \text{---} \alpha \text{---} \beta \text{---} \bullet \xrightarrow{*} \bullet \text{---} \alpha \text{---} \beta + \pi \text{---} \bullet \quad (1)$$

Otherwise, none of the vertices are Paulis; there are 16 line graphs of this form; by Lemma 4.6 these are partitioned in four equivalence classes. Each of the four equivalence classes contains an element of \mathcal{C}_1 , hence $t_1 \xleftrightarrow{*} c \in \mathcal{C}_1$.

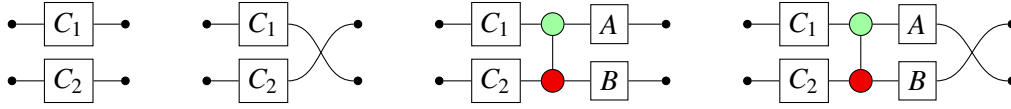
Finally, suppose $n \geq 4$. If t_1 has any Pauli vertices, then $t_1 \xleftrightarrow{*} t_2$ by (1) where t_2 has strictly fewer Pauli vertices, and strictly fewer vertices overall. Otherwise, t_1 has no Pauli vertices; therefore any sequence of vertices of length three can be rewritten, using Lemma 4.6, to a sequence with the colours exchanged. Then by applying the spider and identity rules, and Lemma 4.5 $t_1 \xrightarrow{*} t_2$ where t_2 is in Pauli standard form and has strictly fewer vertices than t_1 . Hence we obtain the result by induction. \square

By enumerating all diagrams with fewer than four vertices, it's easy to check that no $c \in \mathcal{C}_1$ is equivalent to a smaller diagram, so these diagrams are the minimal forms for \mathcal{C}_1 .

4.2 2-Qubit Cliffords

Let \mathcal{C}_2 be the set of diagrams defined in Figure 4. Notice that \mathcal{C}_2 has $24^2(1 + 1 + 9 + 9) = 11520$ elements. As in the case of \mathcal{C}_1 , all the elements of \mathcal{C}_2 are evidently circuits, and it can be mechanically checked that they are all distinct under the standard interpretation. Hence we adopt \mathcal{C}_2 as the normal forms for \mathcal{C}_2 . Again, by the completeness of the axioms (Thm 4.3) we can immediately conclude that every 2-qubit Clifford circuit is equivalent to some $k \in \mathcal{C}_2$. Zooming in a little closer we have the following:

Proposition 4.7. *Let $k \in \mathcal{C}_2$ and let g be a generator of \mathcal{C}_2 as a ZX-calculus term; then $g \circ k \xleftrightarrow{*} k'$ for some $k' \in \mathcal{C}_2$.*



where $C_1, C_2 \in \mathfrak{C}_1$, $A \in \mathfrak{A}$ and $B \in \mathfrak{B}$.

$$\mathfrak{A} = \{ \bullet \text{---} \bullet, \bullet \text{---} \oplus \text{---} \bullet, \bullet \oplus \text{---} \oplus \text{---} \bullet \} \quad \mathfrak{B} = \{ \bullet \text{---} \bullet, \bullet \text{---} \oplus \text{---} \bullet, \bullet \oplus \text{---} \oplus \text{---} \bullet \}$$

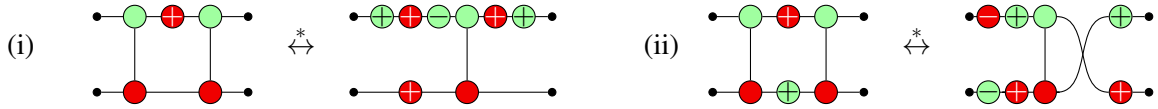
Figure 4: \mathfrak{C}_2 : standard minimal forms for two-qubit Cliffords

Proof. Notice that the 1-qubit Cliffords C_1 and C_2 which occur in k play no part in the computation, hence we ignore them.

There are effectively four choices for g : $(u \otimes \text{id})$, $(\text{id} \otimes u)$, CNOT, or σ , where u ranges over the generators of \mathfrak{C}_1 . If $g = \sigma$, the result is trivial.

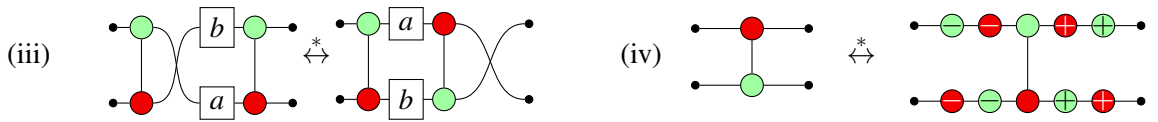
Further, for any $u \in \mathfrak{C}_1$, we have $(u \otimes \text{id}) \circ \text{CNOT} = (a \otimes \text{id}) \circ \text{CNOT} \circ (u_1 \otimes u_2)$ for some $u_1, u_2 \in \mathfrak{C}_1$ and $a \in \mathfrak{A}$, either by commuting vertices of the same colour, or taking out factors of Paulis. Similarly $(\text{id} \otimes u) \circ \text{CNOT} = (\text{id} \otimes b) \circ \text{CNOT} \circ (u_1 \otimes u_2)$ for some $b \in \mathfrak{B}$. Hence the only non-trivial cases to consider are:

1. $g = \text{CNOT}$ and $k = (a \otimes b) \circ \text{CNOT}$. There are nine possibilities for this case, of which we consider two here. If $a = x_+$ and $b = \text{id}$, then by using the bialgebra rule we reduce as shown in (i) below. If $a = x_+$ and $b = z_+$, then a similar argument yields (ii).



They remaining cases can all be derived from these two, except the case where $a = b = \text{id}$, which is trivial.

2. $g = \text{CNOT}$ and $k = (b \otimes a) \circ \sigma \circ \text{CNOT}$. In this case we have (iii) below. However, by exploiting the H rules we have the equivalence (iv) so this case can be reduced to the previous one.



3. $g = \text{CNOT}$ and $k = \sigma$. Again we can apply (iv).

□

As in the single qubit case these reductions will provide the basis for the rewrite rules of our optimiser.

5 Quantomatic

We briefly sketch the Quantomatic system; for a full description see [18]; to obtain it, see [17].

Quantomatic is an interactive theorem prover which can prove equations between terms of the ZX-calculus. The user draws the desired term in the graphical editor, and builds the proof by applying *rewrite*

rules to the current graph. A rewrite rule is a *directed* equation, i.e. a pair of graphs which have the same boundary. Rules are applied in two-step process. First the system searches for subgraphs of the term which are isomorphic to the LHS of the rule; each such subgraph is called a *match*. Quantomatic displays all the possible matches of the chosen rule in the current term, and allows the user to select where the rule is to be applied. The matched subgraph is then replaced by the RHS of the rule to produce a new term. A proof therefore consists of a sequence of terms linked by the application of a particular rule at a particular location in the term.

Quantomatic allows the user to define automated proof tactics, known as simplification procedures or *simprocs*. The name is slightly misleading since there is no need for a simproc to actually *simplify* the graph, in the sense of reducing the number of vertices or edges; however failure to do so will typically result in non-termination. Simprocs are written in the Python programming language, interpreted by the built-in Jython interpreter [1], and augmented with various tactic combinators. The most useful of these are:

- `REWRITE(r)` : given a rule r , apply the rewrite to the first match found.
- `REWRITE_METRIC(r, m)` : given a rule r and a *metric* function $m : \mathbf{ZX} \rightarrow \mathbb{N}$ apply the rewrite to the first match found which *reduces* the metric.
- `REWRITE_TARGETED(r, v, t)` : given a rule r , a vertex v in the LHS of the rule, and a *targeting* function $t : \mathbf{ZX} \rightarrow \text{Vert}$ apply the rewrite r to the first match where vertex v of the rule is matched to the vertex $t(G)$ in the term.

All of these combinators can also accept a list of rules, in which case the rewrites are attempted in the order of the list. Simprocs can be combined in sequence, and also using the combinator `REDUCE(s)` which repeats the simproc s until no new rewrites can be performed.

An important point is that when multiple matches are obtained, the system will select one without user intervention. Which rewrite is selected depends on the internal representation of the term, and is effectively non-deterministic.

The axioms of the ZX-calculus, considered as a rewrite system, are neither terminating nor confluent: for example, if $G \rightarrow G'$ via the π -commute rule then the rule can be applied again immediately to rewrite $G' \rightarrow G$. This and similar cases can easily lead to a non-terminating rewrite strategy. Further although many of the axioms can be oriented in a direction which reduces the graph complexity, the resulting rewrite system is no longer complete with respect to the standard interpretation: in some cases it is necessary to increase the graph size to derive a desired equation.

6 Optimising Clifford Circuits with Quantomatic

In this section we describe our optimisation procedure and summarise the results. The reasons for our choices are discussed in the following section.

By *circuit* we mean a ZX-calculus term which is the image of the translation functor $T : \mathbf{Cliff} \rightarrow \mathbf{ZX}$ defined in Section 4. Note that since \mathbf{Cliff} is a \dagger -PROP and $\llbracket \cdot \rrbracket$ is a strict monoidal functor, the circuits form a sub-PROP of \mathbf{ZX} : they are closed under composition and tensor product; however they are not closed with respect to the equivalence relation $\overset{*}{\leftrightarrow}$.

Most ZX-calculus terms are *not* circuits: some of these don't correspond to Clifford unitaries, and so do not concern us, however there are many non-circuits which are equivalent to circuits via rewriting. We don't attempt to find circuit forms for such terms. Rather, knowing that the input is a circuit, we use rewrites which replace circuits with circuits, and thus stay at all times within the class of circuits.

The axioms of the ZX-calculus are mostly equations between graphs which are evidently not circuits. Therefore our first step is to derive new equations between circuits which will serve as rewrites for use in the main simproc. These rules are listed in Appendix D.

While the derived rules are “obviously” equations between circuits, the circuit structure of a larger graph may not be apparent by looking at a local subgraph. It’s necessary to look at the entire graph in order to guide the rewrite engine.

Definition 6.1. A ZX-calculus diagram is called *simple* if it satisfies the following criteria:

- It is a simple graph.
- No vertex is adjacent to a vertex of the same colour.
- Every degree 2 vertex has a non-zero label.

Lemma 6.2. *Every ZX-calculus diagram is equal to a simple one.*

Proof. Starting with an arbitrary diagram d , first replace all H boxes using the H-euler rule. Then apply the spider rule to fuse spiders, the hopf rule to remove parallel edges, the anti-loop rule to remove any self loops, and the identity to remove trivial spiders everywhere. \square

Definition 6.3. [9] Given a diagram d , with vertices V , inputs I , and outputs O , a *causal flow* (f, \prec) on d consists of a function $f : I + V \rightarrow V + O$ and a partial order \prec on the set $I + V + O$ satisfying the following properties:

- (F1) $f(v) \sim v$
- (F2) $v \prec f(v)$
- (F3) If $u \sim f(v)$ then $v \prec u$

where $v \sim u$ means that u and v are adjacent in the graph.

In the one-way model [24], the existence of a causal flow on a graph implies that measurement-based quantum computation on the corresponding graph state is deterministic [9]. It plays a similar role for ZX-diagrams.

Definition 6.4. A simple ZX-diagram is called *circuit-like* if has the same number of inputs and outputs and its underlying graph admits a *causal flow*.

Proposition 6.5. *Every circuit-like diagram corresponds to a quantum circuit.*

Proof. Using the given flow (f, \prec) we will translate a circuit-like diagram d into a circuit c such that c is obvious in the image to of T .

We must first determine which edges in the diagram correspond to qubits and which correspond to interactions between qubits. Note that for each input i , the flow function f defines a path through the diagram $i \rightarrow f(i) \rightarrow f(f(i)) \rightarrow \dots$. By (F2) and the fact that \prec is a partial order, such a path must terminate at an output; and by (F3) each such input-to-output path is disjoint. Further, since the numbers of inputs and outputs are the same then every vertex of the diagram must occur on one such path.

Now we translate the vertices into gates tracing along the qubit paths. If the vertex has degree 2 it immediately yields a Z_α or an X_β gate. If vertex v has higher degree, let its neighbours, excluding its immediate predecessor and successor, be u_1, \dots, u_n . We decompose v into v_0, v_1, \dots, v_n as shown below:



Note that the new vertices must be compatible with the original ordering, in the sense that if $u_i \sim v \sim u_j$ where $u_i \prec u_j$ then we require that $v_i \prec v_j$. By the flow conditions, none of the u_i belong to the same qubit as v , and by the simplicity of the diagram all the u_i are the opposite colour to v . Note that the updated diagram also admits a causal flow, obtained from the original one in the obvious manner. Hence all the higher degree vertices may be decomposed in the same way, to leave the diagram with no vertex of higher degree than three, and non-zero phases only in the degree two vertices. Then all the links between qubits maybe replaced by CNOT gates; since \prec defines a partial order on the vertices, we are guaranteed this is well-defined. \square

Intuitively the flow path cover specifies which edges of the ZX-diagram are the “qubits” of the circuit; those edges not in the path cover define a CNOT acting on two qubits. Assuming that the graph is a circuit, the path cover is relatively easy to compute by starting at each input and finding a successor among its neighbours. If there is ever a choice of successor for a given vertex this choice can be resolved by looking at the other wires. This information is needed frequently by our optimisation procedure. If an unambiguous path cover cannot be constructed then the procedure halts with an error – in this case the input graph was not a circuit.

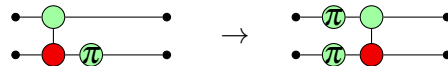
Our optimiser can be summarised as the repeated alternation of two phases:

- Simplification: apply everywhere possible a strictly reducing set of rules.
- Commutation: using targeting and metric rewrites, apply reversible rules to (i) move Pauli operators closer to the inputs. (ii) move CNOT and TONC gates which act on the same two qubits closed together.

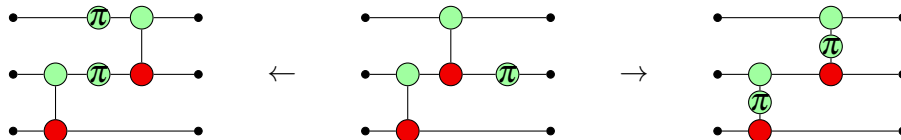
In order to reduce the number of rules, there is an initial phase which replaces all Hadamard, $Z(-\frac{\pi}{2})$ and $X(-\frac{\pi}{2})$ gates with S, V and Paulis as appropriate. The single qubit gates are then “tidied up” by a final pass.

The simplification phase is straightforward, exploiting the different cases of 4.7 as the key rules. The commutation phase is more delicate, and makes heavy use of the path cover computation.

For the single-qubit commutation rules we use targeting function which traverses each path starting from the input and applies the rule at the first possible position in the graph. This works very well and, in concert with the simplification rules, is guaranteed to reduce all single qubit Cliffords to one of the forms of \mathcal{C}_1 . However this approach fails for rules where a Pauli must commute with a CNOT gate. The REWRITE_TARGETED method allows the user to identify a single vertex in the rewrite rule with a single vertex in the graph to be matched. However this is rarely sufficient to uniquely determine the overall match. For example, the following rule



can be applied in two different ways to the central diagram below:



Note that the righthand rewrite does not produce a circuit. The current implementation provides no direct way for a simproc to specify that one matching should be preferred to another, even when it has the

width	depth	input size	output size	size reduction	proof steps	time $\pm \sigma$
1	20	10.8	2.4	0.26	19.6	7 ± 3
2	20	30.2	9.0	0.30	78.9	1021 ± 680
3	20	44.2	14.7	0.32	148	3144 ± 2189
5	20	78.5	22.6	0.28	239	6679 ± 3091

Table 1: Summary of results on randomly generated circuits. Random circuits were generated with the program `randomCliffs.py` which is available from the project repository. Tests were performed on a basic desktop PC.

necessary information. For this reason, we have defined a metric which favours graphs where the Paulis are nearer to the inputs, and maximally penalises graphs with vertices which are not in any path.

The approach sketched here is very conservative: the optimiser only performs rewrites which result in diagrams which meet the (also very conservative) definition of circuit, even in cases where that diagram could be later rewritten to circuit.

7 Summary of results and discussion

Since we have formalised circuits in the ZX-calculus, our measure of size is the number of non-trivial vertices in the graph. This quantity is the gate count over the generating set S, Z, V, X , and CNOT, although each CNOT contributes 2 to the measure. A less obvious consequence of the ZX-calculus formalism is that the swap gate is not represented at all, and CNOT gates may act on any qubits without penalty. This may or may not be realistic for a given quantum architecture, but it is a fundamental feature of the ZX-calculus, and removing it would require a string diagrammatic formalism that takes into account the planarity of diagrams. This would take us far beyond the scope of this work.

Our optimiser reduces all one- and two-qubit circuits to elements of \mathcal{C}_1 and \mathcal{C}_2 respectively; however in larger circuits it does not always find a minimal form. Notably our ruleset does not include any reductions for circuits of three or more qubits, so there are relatively simple CNOT circuits which cannot be reduced. Further, due to the extreme conservativity of our metric and targeting procedures, the optimiser does not always find valid rewrites among the ruleset. However, on a test set of randomly generated Clifford circuits it typically produces significant reductions of circuit size; see Table 1.

There is striking increase in compute time per proof step as the width of the circuit increases. This can be attributed to the increased number of CNOT gates: as the average vertex degree increases, the number of candidate matches including a given vertex increases geometrically. Since many of these matches will be invalid as circuit rewrites, a lot of time is spent searching for matches which are then rejected. Further, wider circuits require two-qubit commutation rules, which are metric-driven rather than targeted, and hence impose a much greater computational load.

Indeed, the main difficulty we have faced is taking control of the matching engine. Targeted rewriting can select good rewrite positions with high efficiency but does not discriminate between good and bad rewrites at that position. Metric-driven rewrites can perform such discrimination but at the cost of losing control over the search. Combining these features in a single combinator would greatly ease this difficulty.

Further, the targeting and metric functors are required to be stateless; this imposes another avoidable performance cost, as the path cover of the graph must be recomputed on every invocation, regardless of whether a rewrite was performed. Given the poor performance of interpreted Python compared to the Scala core, significant speed-up could be achieved by providing a range of built-in metrics for use in

simprocs.

8 Conclusions and Future Work

Since Quantomatic was designed for interactive use, its simproc environment is currently quite limited. In repurposing the system to operate as a fully automated circuit optimisation tool, we have run up against its current limits, and our frequent resort to brute force and perversity is a reflection of these limitations, rather than the authors' mental states⁴. These limitations are not fundamental, and could be removed by minor extensions of the simproc API. Although there is much scope for improvement in our optimiser, we have demonstrated that the Quantomatic system can serve as the basis for an effective circuit optimisation tool.

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⁴However the first author's mental state did take a beating from the lack of debugging facilities.

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A Electronic Resources

All the work described in this paper is available as a downloadable quantum project from the following URL.

<https://gitlab.cis.strath.ac.uk/kwb13215/Clifford-Quanto/>

Please download it and play around!

B An aside on CNOT and SWAP

We have already seen the ZX-calculus representation of CNOT in Section 4. Note that the upper (z) vertex corresponds to the control qubit, while the lower (x) is the target qubit. We could also consider the CNOT with control and target reversed, which we denote TONC.

$$\text{TONC} := \text{Diagram 1} = \text{Diagram 2}$$

The diagram shows two equivalent representations of TONC. The first is a CNOT gate where the control qubit (green dot) is at the bottom and the target qubit (red dot) is at the top. The second is a CNOT gate where the control qubit (red dot) is at the top and the target qubit (green dot) is at the bottom.

It is a well known fact that the swap itself can be represented as $\text{CNOT} \circ \text{TONC} \circ \text{CNOT}$, and indeed this is provable in the ZX-calculus.

$$\text{Diagram 1} \stackrel{*}{\leftrightarrow} \text{Diagram 2} \stackrel{*}{\leftrightarrow} \text{Diagram 3} \stackrel{*}{\leftrightarrow} \text{Diagram 4} \tag{2}$$

The diagram shows a sequence of four diagrams connected by double-headed arrows with an asterisk. The first diagram is a swap gate (two crossing lines). The second diagram is a CNOT gate followed by a TONC gate. The third diagram is a TONC gate followed by a CNOT gate. The fourth diagram is another swap gate.

Note that the bialgebra rule gives the first equation, and the Hopf rule the second: we cannot rely purely on the group structure.

Alternatively, by the colour duality principle we can express TONC in terms of CNOT and H :

$$\text{Diagram 1} \stackrel{*}{\leftrightarrow} \text{Diagram 2} \stackrel{*}{\leftrightarrow} \text{Diagram 3} \tag{3}$$

The diagram shows three equivalent representations of TONC. The first is a TONC gate. The second is a CNOT gate with two H gates on the control qubit. The third is a CNOT gate with two H gates on the target qubit.

Combining (3) and (2) we obtain:

Lemma B.1.

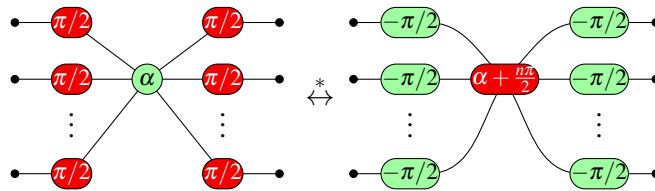
$$\text{Diagram 1} \stackrel{*}{\leftrightarrow} \text{Diagram 2}$$

The diagram shows a swap gate equivalent to a CNOT gate where both control and target qubits have phase shifts of π on the target qubit lines.

Lemma B.1 indicates that we can dispense with the swap as well as TONC and work purely with CNOT. Since we have formalised the system as a PROP it is more convenient to treat σ as one of the generators of \mathcal{C}_2 .

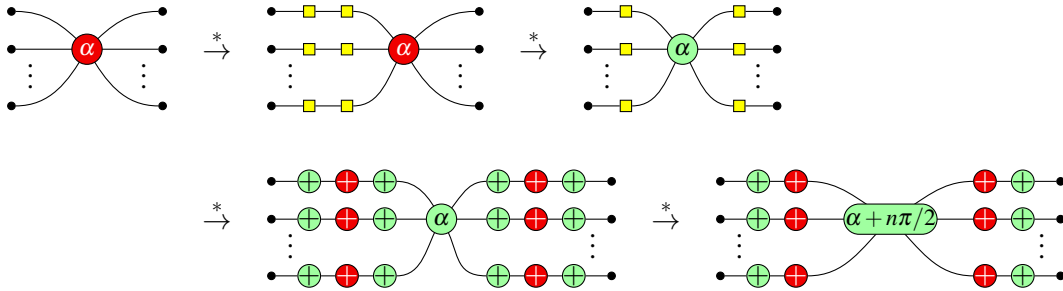
C Proofs omitted from main article

Lemma 3.5 The following rule is admissible:



where n is the number of red vertices in the left hand side diagram.

Proof. Consider a single red spider. By the H-rules, and the spider we may reason as follows:

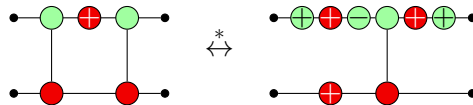


From which the result follows by applying z_- to every leg. □

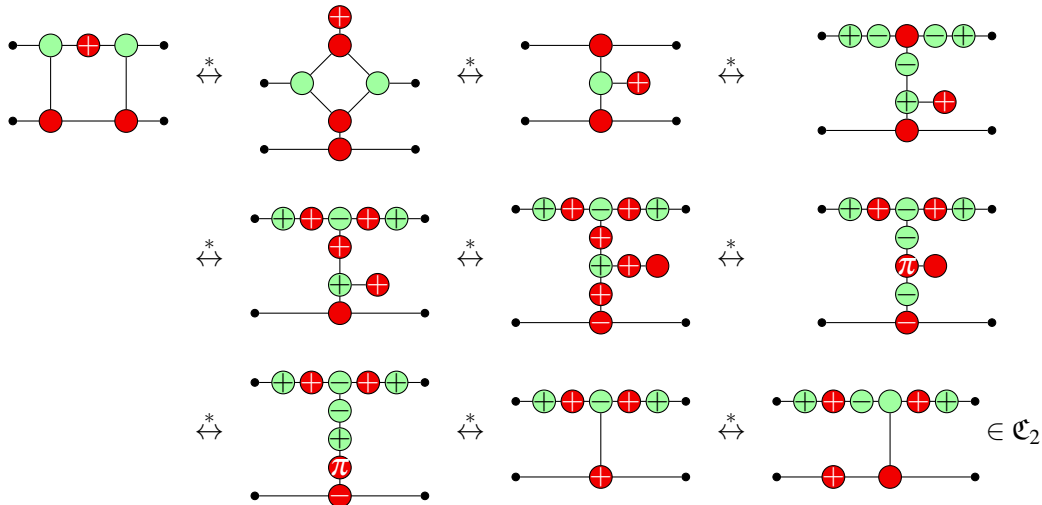
Proposition 4.7 Let $k \in \mathcal{C}_2$ and let g be a generator of \mathcal{C}_2 as a ZX-calculus term; then $g \circ k \xrightarrow{*} k'$ for some $k' \in \mathcal{C}_2$.

Here we fill in the missing details behind the equations (i) – (iv) that appeared in the proof.

Equation (i):

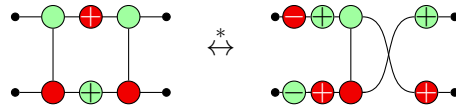


Proof.

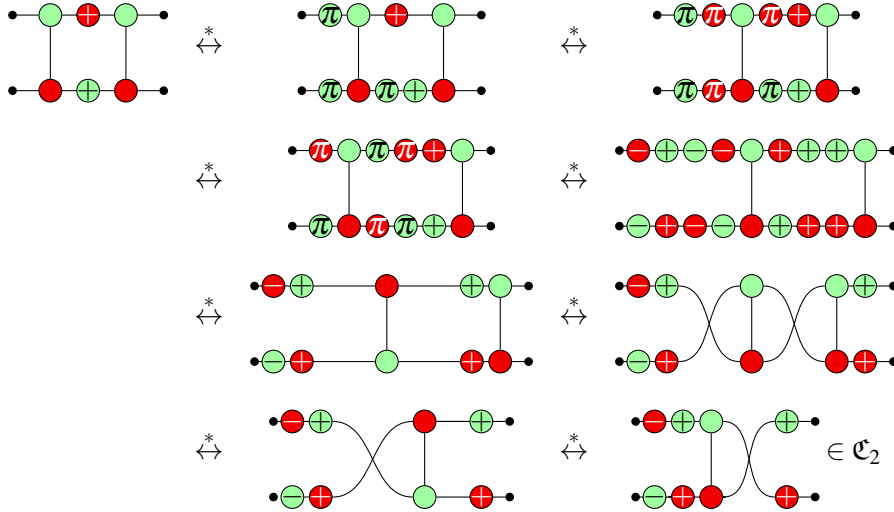


□

Equation (ii):



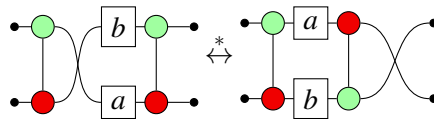
Proof.



Note that we have used both Equations (2) and (3) in the heart of this proof.

□

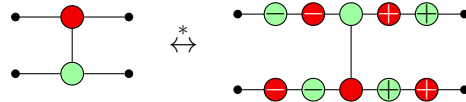
Equation (iii):



Proof. This is a straightforward application of the “topology” principle; no rules are required, they are equal in the sense of Definition 3.1.

□

Equation (iv):



Proof. This is simply Equation (3) from the preceding section.

□

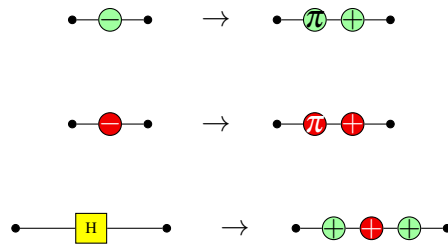
D Main Rules

The following derived rules are the core of the circuit transformations in the main proof development. The rules themselves are found in `derived-rules/` in the Quantomatic project, and their derivations are found in `derived-rules-proofs/`.

In all diagrams inputs are to the left, outputs to the right.

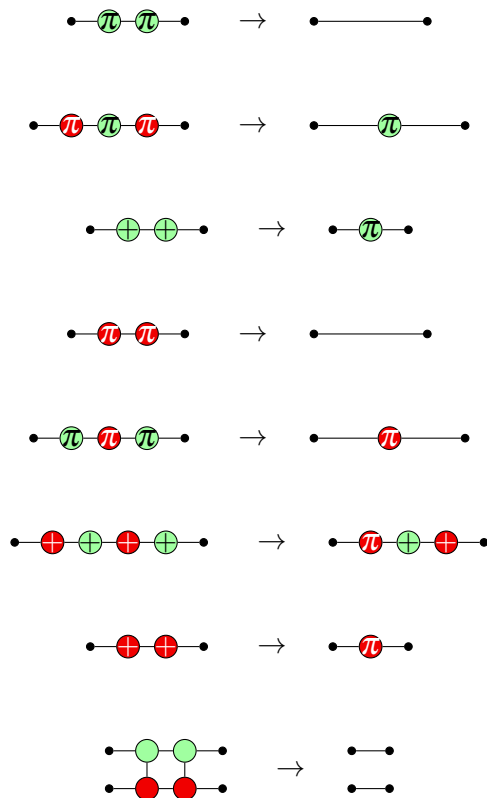
D.1 Init

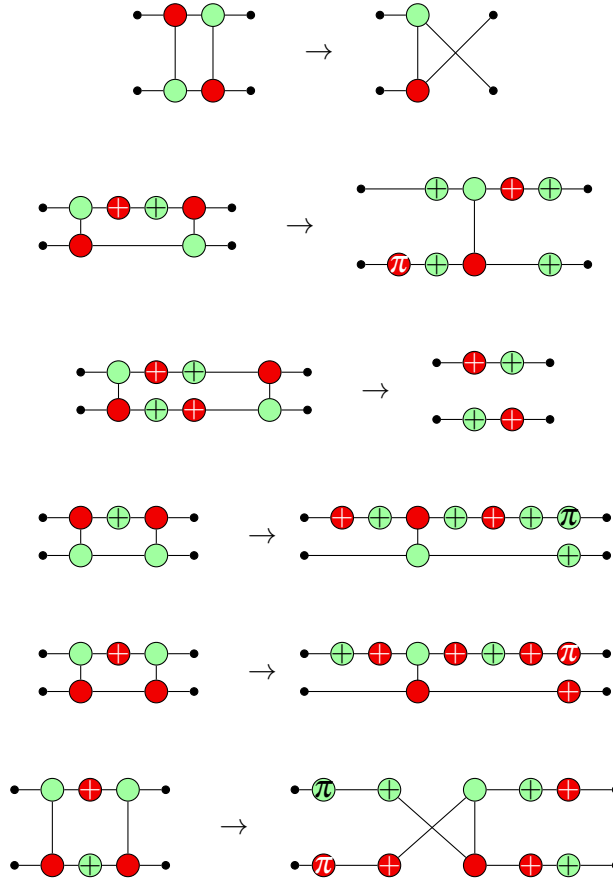
These rules remove all minus and H nodes from the graph.



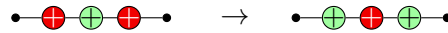
D.2 Always Rules

These are strictly reducing so can always be applied.





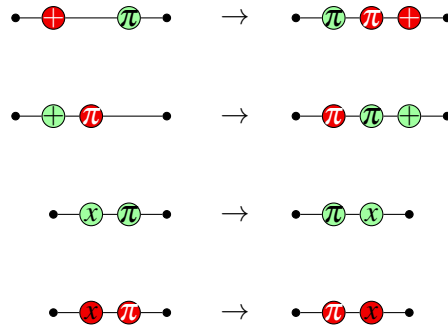
D.3 EulerProc



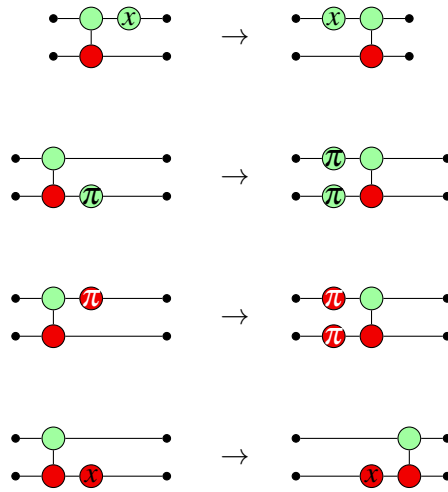
The inverse is also used.

D.4 Pauli Commutation rules

Each of these is managed by a custom simproc which searches for a good place to apply them.



These rules are used by the Pauli Commutation proc, which is based on REDUCE_METRIC.



D.4.1 C2 Rules

These two alternate in the C2Proc simproc. Both have a custom targeting routine to select where they should be applied.

