Towards Minimality of Clifford+T ZX-Calculus



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Abstract

ZX-calculus is a high-level graphical language used for quantum computation. A complete set of axioms for ZX-calculus has been found very recently. This thesis works towards minimizing axioms of ZX-calculus for Clifford+T quantum mechanics, a fragment consisting of an approximately universal gate set. Similar work has been done for the smaller fragment, stabilizer quantum mechanics, which motivates many of our proofs. We derive some singleton axioms and instances of axiom schemes. We establish the necessity and some weaker independence results of several axioms, by considering a variety of models. As a further step towards simplification we also consider alternative presentations of axioms that are equivalent and discuss their uses.

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Chapter 1

Introduction

1.1 History and Motivation

Early stages of the development of quantum mechanics focused on its mathematical and classical physics aspect. It has lead to many difficulties in understanding phenomenons such as entanglement and in reasoning about properties such as non-locality. Approaching quantum theory from a computational perspective then opened up many possibilities, including quantum teleportation [6], factoring algorithm [36], quantum cryptography protocols such as E91 [20] and quantum computation models such as quantum turing machine [15], circuit model [16] and measurement based quantum computing [34]. One of the essential reasons behind the discoveries is the focus on compound states and processes between them, rather than states in isolation. They all exploit the non-classical properties of quantum theory, treating the paradoxes, or bugs, as features.

This sequence of discoveries brings back foundational questions about quantum theory. In particular, it points to the question of whether the Hilbert space model, despite it's correctness, is the best mathematical model for quantum theory. Indeed, quantum theory as modelled by Hilbert space is generally perceived as unintuitive, even in von Neumann's original formulation [38] and the EPR paper [19].

Abramsky and Coecke [1] proposed a more abstract model of quantum theory – the compact closed category. The adoption of category theory puts processes (morphisms) as the main subject of study. The axiomatic setting allows us to understand properties established by quantum theory better. For example, protocols such as quantum teleportation and entanglement swapping can already be realised within the category.

The categorical framework also makes it easier to examine the axioms of quantum theory and compare them with other categories [22], [7], something that is difficult with the very ad hoc Hilbert space model. Indeed, it was realised that the simple category of relation already has many quantum-like features [37] [10].

The categorical approach was then taken a step further, and a graphical calculus, the ZX-calculus, was developed [9]. It was motivated by Penrose [32], who used a graphical calculus as an alternative, informal notation for the tensor notation. Category theory indeed formalizes graphical calculus, so that it is both intuitive and mathematically rigorous. This change from the one-dimensional syntax, that is ordinary algebra as used in Hilbert space formalism, to the two-dimensional syntax, that is equations of diagrams, means that topology and algebra are merged at the syntactic level. One of the major advantage is that equations and theorems of ZX-calculus have a much clearer conceptual and operational meaning. For example, the common protocols as well as quantum gate such as CNOT and Toffoli all take simple forms in ZX-calculus.

The fact that compact closed category works well as a model is perhaps not too surprising, since category theory is already closed linked with other areas of theoretical computer science, for example cartesian closed category for classical computation by the Curry-Howard-Lambek correspondence. However, it is more surprising that the graphical calculus works so well, that quantum gates and circuits appear naturally in the syntax. Evidence of its usefulness has been demonstrated in the recent progress of simplifying quantum circuits using ZX-calculus [13].

In one line, we can argue that the ZX-calculus model is simultaneously more natural to quantum theory and more useful for quantum computation.

It has been ten years since the birth of the ZX-calculus. One of the major tasks was to find a complete set of axioms (in addition to the axioms of compact closed category), so that ZX-calculus can be used completely independently as a model for quantum theory and quantum computation. ZX-calculus comes with a standard interpretation that associates any ZX-diagram with a linear map, and completeness means that any equation of linear maps holds if their diagrammatic presentations can be proved equal. Directly aiming towards a full completion was extremely difficult, and attention has been focused on various fragments. ZX-calculus is a diagrammatic language parameterized by angles in $[0, 2\pi)$, and therefore one gets fragments of the calculus by restricting angles.

The $\frac{\pi}{2}$ -fragment of ZX-calculus has been completely by [2], [3]. This is a restriction of the allow angles to be integer multiplies of $\frac{\pi}{2}$. This fragment of ZX-calculus corresponds to the stabilizer fragment of quantum mechanics in quantum computation literature. This is a promising result towards full completeness, but its practical usefulness is limited since the stabilizer fragment is efficiently classically simulable.

Very recently, [24] and [30] have succeeded in completing ZX-calculus for the $\frac{\pi}{4}$ -fragment of ZX-calculus. This corresponds to the Clifford+T fragment quantum mechanics, which is the most common framework considered for quantum computation, because this fragment is approximately universal for quantum circuits. At the same time, completion of universal ZX-calculus for pure qubit quantum mechanics is done in [29].

A natural further step is to simplify the set of axioms. This is the main subject of study in this thesis. One aspect is to prove the independence of the axioms, and hence aim towards a minimal set of axioms. In other foundational subject with an axiomatic framework, for example set theory, independence proof has been one major area of research. Proofs of several axioms in the $\frac{\pi}{2}$ -fragment of ZX-calculus has been done in [4], [5]. There are still a few open questions in that fragment regarding independence. We are the first to investigate independence and necessity of axioms for the $\frac{\pi}{4}$ fragment. Aiming towards minimality allows us to understand quantum theory better, in that a minimal set of axioms can be seem as the fundamental properties that give rise to all the quantum features. Moreover, minimality means a smaller number of derivation rules required in automatic graphical reasoning tool such as Quantomatic [27], which can potentially significantly speed up the derivations.

Another aspect is to make each individual axiom simpler, which can often be subjective. In terms of our graphical axioms, this can be reducing the number of nodes in one axiom, using diagrams and axioms that have a clearer meaning and find equivalent subsets of axioms. We consider all of these three aspects.

1.2 Outline

The outline of the thesis is as follows:

- 1. In chapter 2, we provide background knowledge.
- 2. In chapter 3, we give some basic and useful properties of the $\frac{\pi}{4}$ -fragment of ZX-calculus which are used. We then give derivations of some axioms, which is the original contribution of this thesis.
- 3. In chapter 4, we approach the task of minimizing the set of axioms for $\frac{\pi}{4}$ -fragment of ZX-calculus. We consider various independence proof methods and prove the necessity of several axioms. All the independence results of axioms of $\frac{\pi}{4}$ -fragment of ZX-calculus is the original contribution of this thesis.
- 4. In chapter 5, we optimize the set of axioms further, by considering different presentations of the axioms.
- 5. In chapter 6, we summarize our findings and give possible directions for future developments.

The specific contributions of this thesis are:

- 1. We derive axioms S2, TR3, L2, L5 and instances of axiom scheme K2, TR13, TR14, L4.
- 2. We show S1, S3, H, IV', AD, L3 are necessary.
- 3. We show some weaker independence results about B1, TR2, TR5', TR6, TR9, TR13 that hints at their possible necessity.
- 4. We present two new generators to give alternative presentations of the axioms.

Chapter 2

Preliminaries

In this section, we provide enough background to make this thesis selfcontained. The main underpinning mathematical subject is category theory. Basic concepts such as category, functor and natural transformation are assumed. We refer to [28] for a most comprehensive cover of the subject. For more related topics in categorical quantum mechanics, we refer to the [23]. A basic understanding of quantum theory and quantum computation would also be helpful, especially in understanding the applications of ZXcalculus and terminologies from quantum mechanics. We refer to [31] for an introduction to the subject.

Oxford Part C courses: Category, Processes and Proofs (CPP), Categorical Quantum Mechanics (CQM) and Quantum Computer Science (QCS) covers everything in Section 2.1 and 2.2.

2.1 Compact closed category

Definition 2.1.1. A category C consists of the following data:

- 1. a collection $Ob(\mathcal{C})$ of objects;
- 2. for every pair of object A, B, a collection $\mathcal{C}(A, B)$ of morphisms, for $f \in \mathcal{C}(A, B)$, we write $A \xrightarrow{f} B$:
- 3. for every object X, an identity morphism $X \xrightarrow{id_x} X$;
- 4. for every pair of morphism $A \xrightarrow{f} B, B \xrightarrow{g} C$, a composite morphism $A \xrightarrow{g \circ f} C$.

In addition, it must have associativity and unit property:

1. associativity: for all morphisms $A \xrightarrow{f} B, B \xrightarrow{g} C, C \xrightarrow{h} D, h \circ (g \circ f) = (h \circ g) \circ f.$

2. unit: for any morphism $A \xrightarrow{f} B$, $f \circ id_A = id_B \circ f$.

Definition 2.1.2. A monoidal category is a category C and in addition has the following data:

- 1. a tensor product functor $\otimes : \mathcal{C} \times \mathcal{C} \to \mathcal{C};$
- 2. a unit object $I \in Ob(\mathcal{C})$;
- 3. a natural isomorphism, the associator $(A \otimes B) \otimes C \xrightarrow{\alpha_{A,B,C}} A \otimes (B \otimes C)$;
- 4. a natural isomorphism, the left unitor $I \otimes A \xrightarrow{\lambda_A} A$;
- 5. a natural isomorphism, the right unitor $A \otimes I \xrightarrow{\rho_A} A$.

which further satisfies certain coherence equations which are called the triangle and pentagon equations:

$$(id_A \otimes \lambda_B) \circ \alpha_{A,I,B} = \rho_A \otimes id_B$$
$$(id_A \otimes \alpha_{B,C,D}) \circ \alpha_{A,B \otimes C,D} \circ (\alpha_{A,B,C} \otimes id_D) = \alpha_{A,B,C \otimes D} \circ \alpha_{A \otimes B,C,D}$$
(2.1)

The naming is from the shape of their commutative diagram, for example the triangle equation can be written as:



Definition 2.1.3. A braided monoidal category is a monoidal category C and in additional has a natural isomorphism $A \otimes B \xrightarrow{\sigma_{A,B}} B \otimes A$, satisfying the two hexagon equations:

$$\alpha_{B,C,A}^{-1} \circ (id_B \otimes \sigma_{A,C}) \circ \alpha_{B,A,C} \circ (\alpha_{A,B} \otimes id_C) \circ \alpha_{A,B,C}^{-1} = \sigma_{A,B \otimes C}$$

$$\alpha_{C,A,B} \circ (\sigma_{A,C} \otimes B) \circ \alpha_{A,C,B}^{-1} \circ (id_A \otimes \sigma_{B,C}) \circ \alpha_{A,B,C} = \sigma_{A \otimes B,C}$$
(2.2)

Definition 2.1.4. A symmetric monoidal category (SMC) is a braided monoidal category C where $\sigma_{B,A} \circ \sigma_{A,B} = id_{A\otimes B}$.

Definition 2.1.5. In a monoidal category C, an object L is left-dual of an object R, and R is right-dual of L, where we denote $L \dashv R$, when there exist a unit morphism $I \xrightarrow{\eta} R \otimes L$ and a counit morphism $L \otimes R \xrightarrow{\epsilon} I$, satisfying equations:

$$\lambda_{L} \circ (\epsilon \otimes id_{L}) \circ \alpha_{L,R,L}^{-1} \circ (id_{L} \otimes \eta) \circ \rho_{L}^{-1} = id_{L}$$

$$\rho_{R} \circ (id_{R} \otimes \epsilon) \circ \alpha_{R,L,R} \circ (\eta \otimes id_{R}) \circ \lambda_{R}^{-1} = id_{R}$$
(2.3)

Note that the existence of duals is a property of a monoidal category. Indeed, if a dual of an object exist, it is unique up to canonical isomorphism.

Definition 2.1.6. A compact closed category (CCC) is a symmetric monoidal category C such that every object has a right dual.

This is the definition as in [1]. There are many other equivalent ways of defining a compact closed category, for example in [26]. In [35] it is also referred to as right autonomous symmetric monoidal category. Directly defining the category being compact (which is essentially the symmetry condition), and closed (which refers to the existence of some internal hom functor that allows currying, and is related to our requirement of objects having duals) is less simple.

One example of a CCC is finite-dimensional vector spaces. To fully model quantum mechanics categorically, we need to have more structure in our category to allow constructions similar to inner products or adjoints in Hilbert spaces.

Definition 2.1.7. A dagger functor for a symmetric monoidal category is a contravariant involutive functor \dagger which sends every object to itself and further satisfies:

$$(g\circ f)^\dagger = f^\dagger\circ g^\dagger ~~(f\otimes g)^\dagger = f^\dagger\otimes g^\dagger ~~\sigma^\dagger_{A,B} = \sigma_{A,B}$$

Definition 2.1.8. A dagger compact closed category, \dagger -CCC, is a compact closed category with a dagger functor \dagger and for every object A (with right dual A^*):

$$\sigma_{A,A*} \circ \epsilon_A^{\dagger} = \eta_{A*}$$

Since we are going to model quantum theory with †-CCC, Hilbert space should be an example of the given category.

Example 2.1.9. The category **FHilb** of finite-dimensional Hilbert spaces is a dagger compact closed category.

- 1. objects are finite-dimensional Hilbert spaces;
- 2. morphisms are bounded linear maps;
- 3. composition is the composition of linear maps as functions;
- 4. identity morphisms are identity functions;
- 5. the tensor product \otimes is the tensor product of Hilbert spaces
- 6. the monoidal unit I is the one-dimensional Hilbert space, C;
- 7. the symmetry isomorphism $\sigma_{H,K} : H \otimes K \to K \otimes H$ is the unique linear map extending $a \otimes b \mapsto b \otimes a, a \in H, b \in K$.

- 8. the dagger functor \dagger : **FHilb** \rightarrow **FHilb** sends morphisms to their adjoints as bounded linear maps.
- 9. Every $H \in \mathbf{FHilb}$ is both right and left dual to its dual Hilbert space H^* .

Note that infinite-dimensional Hilbert spaces do not have duals, hence the more general **Hilb** is not a †-CCC.

2.2 Graphical calculus

It should appear that many conditions in the definitions in the previous section are unintuitive. Manipulating calculations and understanding equations are therefore difficult. This syntactic inconvenience arises essentially because we are squeezing all the algebra into one line, when there are two types of composition(\circ and \otimes). Unambiguity is achieved by using brackets. However, if we adopt a two-dimensional graphical calculus, such syntactic burden disappears.

For a monoidal category, we write morphisms $A \xrightarrow{f} B, B \xrightarrow{g} C, C \xrightarrow{g} D$ as a box with an input and an output wire, each labelled with corresponding object. Composition $g \circ f$ is to connect g on top of f. This is simply rewrite our standard syntax vertically. However, we now write $f \otimes h$ as two boxes side by side, f on the left of g.



Identity is simply a wire with no box in the middle. The monoidal unit I object is not depicted. The identity of I is an empty diagram. At this point, ambiguity might arise, since both $I \otimes A \xrightarrow{\lambda_A} A$ and $A \otimes I \xrightarrow{\rho_A} A$ are depicted as a single wire, while their types are different. The coherence theorem of monoidal category resolves the issue.

Theorem 2.2.1 (Coherence). Any two well-typed morphisms built from

$$\alpha, \alpha^{-1}, \lambda, \lambda^{-1}, \rho, \rho^{-1}, id, \otimes, \circ$$

are equal.

Moreover, consider the interchange law for monoidal category.

Theorem 2.2.2 (Interchange law). For morphisms $A \xrightarrow{f} B, B \xrightarrow{g} C, D \xrightarrow{h} E, E \xrightarrow{j} F$,

$$(g \circ f) \otimes (j \circ h) = (g \otimes j) \circ (f \otimes h).$$

The law is about rebracketing between \circ and \otimes , and one can expect to apply it many times in a derivation. However, in our graphical calculus, the theorem states:



which is trivial and have to hold. Therefore, we have traded an extra dimension with some complexity of one-dimensional syntax. All of these indicate that graphical calculus is really the more natural syntax for monoidal category. The connection between topology and categorical algebra can be strengthened further, according to the correctness theorem, which makes the graphical calculus rigorous.

Theorem 2.2.3 (Correctness of monoidal category graphical calculus). A well-typed equation between morphisms in a monoidal category is derivable from the axioms (of monoidal category) if and only if it holds in the graphical calculus up to planar isotopy.

Graphical calculus can be extended even further. For symmetric monoidal category, we denote $\sigma_{A,B}$ as two wires swapping, and the condition in the definition, looks like:



Types are omitted since it's clear from context. We also have the correctness theorem for SMC.

Theorem 2.2.4 (Correctness of SMC graphical calculus). A well-typed equation between morphisms in an SMC is derivable from the axioms if and only if it holds in the graphical calculus up to four-dimensional isotopy, equivalently, graph isomorphism.

For duals, we depict unit and counit morphisms (again omitting types) as:



and the conditions become:

•

Therefore for the graphical calculus for a CCC is the same as an SMC, with the extra cups and caps satisfying the above equations that we can use. For a dagger functor, we depict the dagger of a morphism as its mirror image, that is:



The graphical calculus of †-CCC is that of CCC and in addition satisfies:



For details of the proofs of the coherence theorems and correctness theorems, as well as many more different categories and their graphical calculi, we refer to [35].

2.3 ZX-calculus

ZX-calculus is a dagger compact closed category, **ZX**. The objects are the natural numbers \mathbb{N} . The tensor on objects is the addition of numbers, $n \otimes m = n + m$. The morphisms are ZX-diagrams. A ZX-diagram $D : k \to l$ with k inputs and l outputs is finitely generated by:



where $n, m \in \mathbb{N}, \alpha \in [0, 2\pi)$, *e* represents an empty diagram.

using the two compositions:

- 1. Spacial composition: for any $D_1 : a \to b$ and $D_2 : c \to d$, $D_1 \otimes D_2 : a + c \to b + d$ is built by placing D_1 on the left side of D_2 .
- 2. Sequential composition: for any $D_1 : a \to b$ and $D_2 : b \to c$, $D_2 \circ D_1 : a \to c$ is built by placing D_1 on top of D_2 , connecting the output of D_1 to the inputs of D_2 in the given order.

Note the construction of sequential composition, that we refer to top ends as inputs and bottom as outputs. So diagrams is read from top to bottom. This became the more common convention during the development of ZXcalculus and is usually opposite to other process theories, and the general definitions we states in Section 2.2. For the morphisms with green and red nodes, we refer to them as (green or red) spiders. We refer to the angles on them as phases. When a phase $\alpha = 0$, we usually omit writing it. We call a diagram a scalar when it has no input and output wires.

We also have the standard interpretation [.], which is a monoidal functor from the category **ZX** to the category **FHilb**. It associates any diagram $D: n \to m$ a linear map $[D]: \mathcal{C}^{2^n} \to \mathcal{C}^{2^m}$ inductively defined as follows:



where $M^{\otimes 0} = (1)$ and $M^{\otimes k} = M \otimes M^{\otimes k-1}$ for any $k \in \mathbb{N}^+$ and matrix M.

Note that we have to define the green dot as a separate degenerate case of green spider. Some example standard interpretation of morphisms are:

$$\begin{bmatrix} \bullet \\ \bullet \end{bmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i\alpha} \end{pmatrix} \quad \begin{bmatrix} \bullet \\ \bullet \end{bmatrix} = (1 + e^{i\alpha})$$
$$\begin{bmatrix} \bullet \\ \bullet \end{bmatrix} = \sqrt{2}e^{i\frac{\alpha}{2}} \begin{pmatrix} \cos(\frac{\alpha}{2}) \\ -i\sin(\frac{\alpha}{2}) \end{pmatrix} \quad \begin{bmatrix} \bullet \\ \bullet \end{bmatrix} = e^{i\frac{\alpha}{2}} \begin{pmatrix} \cos(\frac{\alpha}{2}) & -i\sin(\frac{\alpha}{2}) \\ -i\sin(\frac{\alpha}{2}) & \cos(\frac{\alpha}{2}) \end{pmatrix}$$

The standard interpretation has significant importance, since it makes a connection between ZX-calculus and FHilb. The universality, soundness and completeness results that we will state are all about relating ZX-calculus with **FHilb**.

Theorem 2.3.1 (Universality). For any linear map $M : \mathbb{C}^{2^n} \to \mathbb{C}^{2^m}$, or equivalently matrix $M \in \mathbb{C}^{2^n} \times \mathbb{C}^{2^m}$, there exist a diagram $D : n \to m$ such that $\llbracket D \rrbracket = M$.

Proof. Proof is given in [9] using Euler-angle decomposition on Bloch sphere and the result from quantum computation that any n-qubit unitary map can be constructed using CNOT and an one-qubit unitary. \Box

In quantum computing terms, we say that ZX-calculus is universal for pure state qubit quantum mechanics. This gives the ZX-calculus enough expressive power. Note that for a matrix of dimension $2^n \times 2^m$, we only need a diagram 'of dimension' $n \times m$. It is essentially because our syntax is truly two-dimensional as the geometry encodes useful information which reduces the dimension needed.

However, to achieve universality we need an uncountable set of angles, $[0, 2\pi)$. Therefore, for practical purpose, we generally consider approximate universality, the ability to approximate any linear map with arbitrary accuracy, using a finite set of angles. The $\frac{\pi}{4}$ -fragment meets the requirement, where we restrict angles to be only multiples of $\frac{\pi}{4}$. In quantum mechanics terminology, this fragment of ZX-calculus corresponds to the Clifford+T fragment of quantum mechanics. The fragments are subcategories of **ZX**.

Clearly, in general, the ZX-diagrammatic representation of a matrix is non-unique. One of the main goal in the development of ZX-calculus is to also equip the calculus with deductive power. That is, adding axioms (equations between morphisms) that we can use to prove equations between diagrams, making ZX-calculus a theory on its own. In logic terms, the task is to look for a sound and complete set of rules, which has been extremely difficult. A complete set of rules for the $\frac{\pi}{4}$ -fragment was first found in [2], [3]. Very recently, a complete set of rules for the $\frac{\pi}{4}$ -fragment was found in [24]. We refer to [24] as the JPV paper. Then, a complete set of rules for whole pure qubit quantum mechanics was found in [29], which is modified into a complete set of rules for $\frac{\pi}{4}$ -fragment in [30] by the same authors. We refer to [29] (or [30] interchangably) as the NW paper. The axioms from the NW paper is the main subject of study in this thesis, we refer to the category with this set of axioms as $\mathbf{ZX}_{\pi/4}$. The axioms involve two new generators, the lambda box λ and the triangle Δ , which we add to the $\pi/4$ -fragment ZX-calculus.



 $\mathbb{Z}[\frac{1}{2}]$ is the ring \mathbb{Z} appending $\frac{1}{2}$. It is exactly the dyadic rationals. So any λ is in the form of a minimal coprime fraction, $\frac{a}{2b}$, $a, b \in \mathbb{N}$.

We also need to extend the standard interpretation [.].



We present the full set of axioms in three parts, which we will constantly refer to: the <u>standard rules</u> in Figure 2.1, the <u>triangle rules</u> in Figure 2.2 and the <u>lambda rules</u> in Figure 2.3. We sometimes write \triangle and λ for simplicity. We state the soundness and completeness result formally.

we state the soundness and completeness result formally.

Theorem 2.3.2 (Soundness). $\mathbf{ZX}_{\pi/4}$ is sound: if $\mathbf{ZX}_{\pi/4} \vdash D_1 = D_2$, then $\llbracket D_1 \rrbracket = \llbracket D_2 \rrbracket$.

Proof. The proof is routine as we simply check that the standard interpretation of two sides of every axiom is equal. \Box

Theorem 2.3.3 (Completeness). $\mathbf{ZX}_{\pi/4}$ is complete: if $\llbracket D_1 \rrbracket = \llbracket D_2 \rrbracket$, then $\mathbf{ZX}_{\pi/4} \vdash D_1 = D_2$.

Proof. For both sets of axioms, in the JPV paper and the NW paper, the completeness proof relies on the completeness result of another graphical calculus for the category of free abelian groups, ZW-calculus, introduced in [21], by defining functors between ZX and ZW. \Box

There are other variations of the definition of completeness too. For example, completeness with respect to Clifford+T circuits, which states any equivalent circuit should be derivable with the set of axioms. We do not consider those and only use completeness with respect to the standard interpretation.



Figure 2.1: The standard ZX rules for $\pi/4$ -fragment. $\alpha, \beta \in \{\frac{k\pi}{4} | k = 0, 1, \ldots, 7\}$. In S1, the number of inputs and outputs on two sides agree. For the namings of axioms: S stands for spider. H stands for hadamard. B stands for bialgebra. EU stands for euler-decomposition. K stands for commute.



Figure 2.2: The triangle rules, for the $\pi/4$ -fragment ZX-calculus. $\alpha \in \{\frac{k\pi}{4} | k = 0, 1, \dots, 7\}$. The namings of the axioms remain from their first version, hence there is gap in numbering and '-symbol for some axioms.



Figure 2.3: The lambda rules, for the $\pi/4$ -fragment ZX-calculus. $\lambda, \lambda_1, \lambda_2 \geq 0, \lambda, \lambda_1, \lambda_2 \in \mathbb{Z}[\frac{1}{2}]$. So $\lambda, \lambda_1, \lambda_2$ are the non-negative dyadic rationals: rationals of minimal coprime form $\frac{a}{2^b}$ where $a, b \in \mathbb{N}$. $\alpha, \beta, \gamma \in \{\frac{k\pi}{4} | k = 0, 1, \ldots, 7\}$. AD stands for addition. In AD, $\lambda e^{i\gamma} = \lambda_1 e^{i\alpha} + \lambda_2 e^{i\beta}$.

Chapter 3

Derivable axioms

In this section, we show some axioms are indeed derivable and therefore can be removed. A general remark is that many of the properties that we state follow from their derivations in $\pi/2$ -fragments. However, not all of them immediately carry over, since the axioms of $\pi/2$ -fragment is not a subset of the axioms of $\pi/4$ -fragment that we presented in Figure 2.1, 2.2, 2.3. This is especially important when we show an axiom is derivable, as we want to make sure all the lemmas we used have proofs that do not used that axiom, so that there is no circular argument.

3.1 The standard rules

Lemma 3.1.1. The common dot decomposition holds.



Note that we can apply any axiom upside down by taking dagger functor. The colour swapped versions of the axioms we used can be obtained using axiom H. As an example first proof we label at each step the axiom used. \Box

Lemma 3.1.2. The Hopf law holds.



(Hopf)

Proof. A proof is given in [?] for $\pi/2$ -fragment. The proof carries over, using graph isomorphism, S3, B2, B1.

Lemma 3.1.3. The inverse rule used in π and $\pi/2$ -fragment, which does not involve phases, is derivable.

$$= \begin{array}{c} & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & &$$

Proof. We refer to [30] for the proof in $\pi/4$ -fragment. Axioms IV, B1, S1, and Hopf law in Lemma 3.1.2 are used.

We now show the first derivable axiom.

Lemma 3.1.4. S2 is derivable.

Proof.



where we uses S3, S1 and axiom of †-CCC.

Note that this proof is subtle, The second step will not work if we have diagrams horizontally flipped.



This is because S1 has the α -node above the β -node. Formally, the outputs of α -node are connected to the inputs of β -node, not the other way round.

Next axiom we investigate is K2. We can view K2 as an axiom scheme for 8 equations, or as having a quantifier.

$$\forall \alpha \in \{\frac{k\pi}{4}, k = 0, 1, \dots, 7\}, \qquad \qquad \bullet \qquad \stackrel{a}{=} \qquad \stackrel{a}{=} \qquad \stackrel{a}{=} \qquad (K2)$$

K2 is known to be derivable for the $\pi/2$ -fragment, and it is believed that K2 is necessary for $\pi/4$ -fragment. We show that rather than having α quantified, only one angle is needed.

Lemma 3.1.5. EU can be replaced with the smaller EU'.

$$= \frac{\pi}{2}$$
(EU')

Proof. It easy to check that EU' is sound. For maintaining completeness, we need to have a derivation of EU from EU'. We refer to Lemma A.16 in [4]. Note that the proof in [4] in the $\pi/2$ -fragment, and uses IV2 from Lemma 3.1.3, and we carefully check that the proof carries over to our set of axioms. The proof uses only axioms from the standard rules.

Lemma 3.1.6. Using EU' instead of EU, K2 is derivable for $\alpha = 0, \pi$.

Proof. Proof is given in [4], which is very long and technical. Again it heavily uses IV2 and EU', which are taken as axioms for the $\pi/2$ -fragment in [4]. We have shown in Lemma 3.1.3 and 3.1.5 that they hold in our $\pi/4$ -fragment. The derivation of K2 is in $\pi/2$ -fragment and carries over to our set of axioms for $\pi/4$ -fragment.

Lemma 3.1.7. Using EU' instead of EU, The green π -phase is copied by red spider.



Proof. Again it is proved in [4]. Its colour-swapped version is obtained by applying hadamard on the outputs. \Box

Lemma 3.1.8. Using EU' instead of EU, for α , β in $\pi/4$ -fragment, we have:



Lemma 3.1.9. Using EU' instead of EU, K2 can be replaced by K2'.



Proof. Since we have Lemma 3.1.6, we just need to show that instances of K2 for $\alpha = 3\pi/4, 5\pi/4, 7\pi/4$ is derivable. For $\alpha = 3\pi/4$,



where in the last step we uses Lemma 3.1.8 and S1. The cases for $\alpha = 5\pi/4, 7\pi/4$ can be shown similarly.

Therefore, rather than being an axiom scheme, K2 can be replaced by singleton axiom K2'. So its important is essentially in expressing a commutation relationship between $\pi/4$ and π phases of opposite colours, and the other commutation relationships will simply follow.

3.2 The triangle rules

Lemma 3.2.1. TR13 can be replaced by TR13- where $\alpha = \pi/4$.



Proof. For instance of a general phase $\alpha = \frac{k\pi}{4}$ simply apply TR13- k times.

Therefore TR13 can be reduced to a singleton axiom, rather than being an axiom scheme, just like K2.

Now we derive TR3.

Lemma 3.2.2. A similar rule to TR2 is derivable.



The last step of derivation uses TR5'.

This lemma turns out to be useful again in deriving L2.

Lemma 3.2.3. Using EU' instead of EU,



Proof. Proof is given for $\pi/2$ -fragment in [4]. We check that the proof indeed carries over.

Lemma 3.2.4. Using EU' instead of EU, TR3 is derivable.

A consequence of Lemma 3.2.3 is that,



Proof.



Step 1 uses S1, step 2 uses TR6, step 3 uses TR2, step 4 uses equation above, step 5 uses Lemma 3.2.2. Note that we should carefully check that the lemmas applied do not use TR3 itself it the proofs. \Box

3.3 The lambda rules

Lemma 3.3.1. *TR14* can be replaced by *TR14-*, which is when we restrict to $\lambda = \frac{1}{2}$ and $\lambda = p$ where p is prime.



Proof. We just need to show that this restricted version can derive TR14 for all $\lambda \in \mathbb{Z}[\frac{1}{2}]$. We can derive TR14 for any $\lambda = \frac{1}{2^k}$ by applying the rule with $\lambda = \frac{1}{2} k$ number of times. For $\lambda = 1$, by L3, the lambda box becomes a wire, and hence TR14- holds trivially. We can derive TR14 for any integer $\lambda = n \geq 2$, since each n has a (unique) prime factorization, $n = p_1 p_2 \dots p_k$,

and we apply the rule with $\lambda = p_i$ for $i \in \{1, \dots, k\}$. Then, since each λ can be expressed in $\frac{n}{2^k}$, using L4, we can derive TR14 for any λ .

So we reduce the parameter space of axiom scheme TR14. However unlike Lemma 3.1.9 and 3.2.1 for K2 and TR13, it is unlikely to reduce TR14 further, even to a finite axiom scheme, essentially because $\lambda \in \mathbb{Z}[\frac{1}{2}]$.

Next we state a useful property about \triangle and λ

Lemma 3.3.2. \triangle and λ can be expressed spiders and hadamards only.



(3.3)

where in the last equation $\lambda = [\lambda] + \{\lambda\}$, that is a sum of its integer and fractional part. The fractional part can be subsequently expressed as sums of integer multiplies of $\frac{1}{2^k}$, i.e. $\{\lambda\} = a_1 \frac{1}{2^1} + \cdots + a_s \frac{1}{2^s}$.

Proof. The first decomposition of \triangle is given as a definition in [24]. The second is given in [11]. It is easy to verify that they hold in our axioms. The decompositions of λ , as a sum of its integer part and its fractional part, is given in [29][30].

The derivation of integer λ uses L3 for base case ($\lambda = 1$) and AD recursively for general n. For $\lambda = \frac{1}{2^k}$, the obvious derivation is to derive the base case of $\lambda = \frac{1}{2}$ using L3, AD and TR14 first, and then use L4 recursively for general $\lambda = \frac{1}{2^k}$. However we can indeed avoid using L4. We can derive a reverse recursive formula, expressing $\frac{1}{2^k}$ using $\frac{1}{2^{k+1}}$:



where step 2 uses TR14, step 3 uses S1 and B1, step 4 uses L1. Then observe that:



where we uses TR5', dot decomposition from Lemma 3.1.1 and IV2 from Lemma 3.1.3. This gives us the recursive formula:



The base case is obtained simply by taking k = 0 and apply L3. Therefore we have the decomposition of $\lambda = \frac{1}{2^k}$ stated in the lemma for any k, without using L4. Hence L4 is only used for a general λ with fractional part not just a power of $\frac{1}{2}$.

Lemma 3.3.3. L4 with
$$\lambda_1 = \frac{1}{2^k}, \lambda_2 = \frac{1}{2^l}$$
 is derivable

Proof. Use the decomposition form of λ_1, λ_2 as given in Lemma 3.3.2 above, and then simply apply S1. As we have just shown, decomposing such λ_1, λ_2 do not require L4, so there is no circular argument.

This is again a similar result to Lemma 3.1.9, 3.2.1, 3.3.1, reducing the parameter space. However it seems like the parameter space can not be easily reduced further. Unlike Lemma TR14-, we can't even restrict integer λ to primes. Following the similar strategy as for the case of λ as power of $\frac{1}{2}$ above lead us to some equation between triangles which does not seem to simplify.

The decomposition of integer λ is not expanded in full. We expand it further into a simpler form.

Lemma 3.3.4. For integer $\lambda = n$, we have:



where in the first step, we recursively substitute the integer expansion, and in the second step TR7 is used n-1 times.

This decomposition of integer λ is more intuitive. It is the 'string of triangle' that provides the value n in the matrix of $\lambda = n$:

Lemma 3.3.5. First equality in L1 is derivable, i.e. we can replace it with axiom L1':

$$\begin{array}{c} \lambda \\ \bullet \end{array} = \begin{array}{c} \bullet \\ \lambda \end{array}$$
(L1')

-

Proof. Simply follows from graph isomorphism which is a consequence of axiom of †-CCC by the correctness theorem.



Lemma 3.3.6. L2 is derivable.

Proof. For integer $\lambda = n$, we have:



Step 1 is by Lemma 3.3.4, step 2 is IV2 from Lemma 3.1.3, step 3 is B2, step 4 is repeatedly TR2, step 5 is IV2.

For $\lambda = 1/2^k, k \in \mathbb{N}$, we have:



Step 1 is by Lemma 3.3.2, step 2 is by IV2 repeated k times, step 3 is by B2 repeatedly, step 4 is by Lemma 3.2.2 repeatedly, step 5 is by Lemma 3.1.1 and then IV2 repeatedly.

Then, for general λ , we express $\lambda = \frac{n}{2^k}$, $n, k \in \mathbb{N}$, using L4 and the above results, we have:



Therefore L2 is derivable. Again, we carefully check that during the derivation of all the lemmas mentioned, L2 itself is not used. \Box

Lemma 3.3.7. L5 is derivable. Proof.



Lemma 3.3.8. TR13 and TR14 can be replaced by one rule, TR13'.



Proof. Clearly TR13' can be derived by applying TR13 first, and then TR14. For the converse, when $\alpha = 0$ it becomes TR14, when $\lambda = 1$ it becomes TR13.

This lemma can clearly be combined with Lemma 3.2.1 and 3.3.1.

To give the most up-to-date conclusions, we also have the following recent results.

Lemma 3.3.9. TR4, TR7, TR10' are derivable. L1' is derivable. Proof. This is a result in Quanlong Wang's PhD thesis [39].

To sum up, in this section we derived axioms S1, TR3, L2, L5 and simplified L1, K2, TR13, TR14, L4. Together with the most recent results in Lemma 3.3.9, the original set of axioms has already been significantly reduced.

Chapter 4

Independence and necessity

Independence proof is one of the most foundational question in any axiomatic theory. We state the methodology used first. In logic terminology, it is to find alternative models of the theory. Since we always want to maintain completeness, we naturally have a notion of necessity of an axiom.

Definition 4.0.1. An axiom A is independent from $\mathbf{ZX}_{\pi/4}$ if $\mathbf{ZX}_{\pi/4} - A \nvDash A$. A. A non-empty subset $S \subseteq \mathbf{ZX}_{\pi/4}$ is independent from $\mathbf{ZX}_{\pi/4}$ if for each $A \in S$, $\mathbf{ZX}_{\pi/4} - S \nvDash A$.

Note that $\mathbf{ZX}_{\pi/4}$ refers to the axioms in Figure 2.1, 2.2, 2.3 plus the axioms of \dagger -CCC.

Definition 4.0.2. Given a functor $\llbracket.\rrbracket' : \mathbf{ZX}_{\pi/4} \to \mathcal{C}$, an axiom $D_1 = D_2$ is satisfied by $\llbracket.\rrbracket'$ if $\mathcal{C} \vdash \llbracket D_1 \rrbracket' = \llbracket D_2 \rrbracket'$. A subset $S \subseteq \mathbf{ZX}_{\pi/4}$ is satisfied if each axiom in S is.

Definition 4.0.3. An axiom A is necessary if $\mathbf{ZX}_{\pi/4} - A$ is not complete.

Lemma 4.0.4. Given a functor $[\![.]\!]'$, if a non-empty subset $S \subseteq \mathbf{ZX}_{\pi/4}$ is the set of axioms not satisfied by $[\![.]\!]'$, then subset S is independent from $\mathbf{ZX}_{\pi/4}$. Therefore at least one axiom in S is necessary.

Proof. Suppose S is not independent from $\mathbf{ZX}_{\pi/4}$. Then there exist $A \in S$, $\mathbf{ZX}_{\pi/4} - S \vdash A$. Consider the proof of A, which is of finite length and at each step, an axiom $D_1 = D_2$ is applied. Each axiom used is not in S, therefore they are satisfied by $[\![.]']$. Therefore we can rewrite the proof in category C, at each step, apply rule $[\![D_1]\!]' = [\![D_2]\!]'$ which holds in C. By induction, A holds in C, which is a contradiction since $A \in S$. Therefore S is independent from $\mathbf{ZX}_{\pi/4}$.

Now suppose none of S is necessary. Then for each $A \in S$, $\mathbf{ZX}_{\pi/4} - A$ is complete. Enumerate S and by induction (which we can do since $\mathbf{ZX}_{\pi/4}$ has countable number of axioms), $\mathbf{ZX}_{\pi/4} - S$ is complete. Since each $A \in S$ is sound, $\mathbf{ZX}_{\pi/4} - S \vdash A$, contradicting the independence of S. \Box

Note that this is the strongest general proof, and we can not conclude each axiom in S is necessary in the above lemma. Therefore, necessity is a stronger property than independence.

However, at a special case necessity and independence coincides, and it will provide the best result that we want.

Lemma 4.0.5. Given a functor $[\![.]\!]'$, if there is exactly one axiom S not satisfied, then it is independent from $\mathbf{ZX}_{\pi/4}$ and is necessary.

Proof. Special case of Lemma 4.0.4 when restricting set S to singleton set. \Box

Therefore the task is to find appropriate categories and functors into them. The categories we will use are:

- 1. Booleans. Since axioms we have are equations of diagrams, the arguments become graph-theoretic. That is, we say a set of axioms is independent because they are the only axioms that can create/eliminate/modify some graph-theoretic property. These independence proofs are a lot easier, but at the same time only applies to the simplest axioms.
- 2. Finite sets. This is investigating parity-related properties of the diagrams.
- 3. $\mathbf{ZX}_{\pi/4}$. Just like models of set theory are often sets, functors other than the standard interpretation that map into $\mathbf{ZX}_{\pi/4}$ will be used.

Necessity has been investigated for the $\pi/2$ -fragment, [4], [5], which motivates many of our constructions. However they all have to be modified and extended. We will use the term functor and interpretation interchangeably.

In the remaining of the chapter, we always state our result in terms of necessity, rather than independence.

4.1 Graph-theoretic proofs

Lemma 4.1.1. Rules S1, H, IV are necessary.

Proof. Follow with essentially the same arguments as in [5] for $\pi/2$ -fragment of ZX-calculus. S1 is the only rule that transform a node of degree ≥ 5 to a diagram containing lower-degree nodes. (AD relates green node with degree 4 on one side to green node with degree 2 on the other, but there's no rule relating green node with degree 5.) H is the only rule that matches red nodes of degree ≥ 4 . IV the only rule that relates the empty diagram.

Lemma 4.1.2. S3 is necessary.

Proof. S2 and S3 are the only rules that transform a wire incident on a node to a wire not incident on a node. Then, since S2 is derivable, we conclude S3 is necessary. \Box

Lemma 4.1.3. Either B1 or TR5' is necessary.

Proof. They are the only rules that transform a diagram with inputs or outputs connected to one disconnected. \Box

Lemma 4.1.4. At least one of TR2, TR5', AD is necessary.

Proof. After removing the derivable rules, they are the only ones that relates a diagram containing triangle to one without. \Box

Lemma 4.1.5. L3 is necessary.

Proof. L2 and L3 are the only rules that relate a diagram containing λ with one that doesn't. Since we showed L2 is derivable, we conclude L3 is necessary.

Note that we need to be careful when reasoning about graph-theoretic property, and sometimes it will be helpful to write down the formal definition of the functor behind our arguments. Doing this for all the above lemmas is overly rigorous. The potential problem is that what counts as a graphical invariant is not entirely obvious, we give a non-example to demonstrate.

Non-example. We might want to assert B1 is necessary, since it is the only rule that relates a diagram with two outputs connected to one with two outputs disconnected. This is indeed the proof given for the necessity of B1 in $\pi/2$ -fragment in [5]. For $\mathbf{ZX}_{\pi/4}$, this is wrong, since we can use TR5' and the cap morphism to obtain a rule:



which defeats the proof above. So the existence of cup and cap states means being an input or output is no longer significant, and it is the connectivity of the entire diagram that matters.

The formal functor will send all morphisms with both inputs and outputs to True, and other morphisms (including the empty diagram) to False, sequential composition to \wedge and spacial composition to \vee . We check that this is indeed a functor. Applying this yields the results in Lemma 4.1.3.

4.2 Parity-based models

Next we investigate parity-based interpretations. $[\![.]\!]^b$ is defined in [5] for the $\pi/2$ -fragment, to show either S3 or B2 is necessary in that fragment. We extend it to the $\pi/4$ -fragment.

Definition 4.2.1. Define interpretation $[\![.]\!]^b$ on red spiders and hadamards as follows:



where $[\![.]\!]$ is the standard interpretation. $[\![.]\!]^b$ on green spiders, wires, empty diagram \triangle and λ are the same as $[\![.]\!]$.

Indeed, since $[\![.]\!]^b$ is from $\mathbf{ZX}_{\pi/4}$ to $\mathbf{ZX}_{\pi/4}$ itself, and only multiplies non-zero scalers to all generators, we can simply define $[\![.]\!]^b$ as functor into set consisting of i, -i, -1, 1, as:



and sends all other generators to 1.

The motivation is that most rules should be sound: when turning some red spiders into green ones in an equation, hadamards arise due to the H rule. This justifies adding nothing to wires and empty diagram. This also justified our definition of having an interpretation that does not distinguish between specific phases.

Now we need to define $[\![.]\!]^b$ on the remaining generators: \triangle and λ . We decide it by looking at their decompositions in Lemma 3.3.2. The sum of degrees of red nodes minus number of hadamards, in the two decompositions of \triangle , are 8 and 10. Since $i^8 = 1$, we define $[\![.]\!]^b$ on \triangle as 1. Later we will consider sending \triangle to $i^{10} = -1$.

For simplicity we send λ to 1 for now. Following the decomposition will give a different value.
It is routine to check that the functor does not satisfy: H2, EU, TR6, IV, and in addition H unless n + m is even. So at least one of H2, EU, TR6, IV, H is necessary.

Now consider variants of the above functor. We try combinations of powers of i, -i, -1 and 1. Difference result will arise since these numbers have different degrees of unity. Again, we define the interpretations of \triangle and λ following the same motivation.

Definition 4.2.2. Let all variants of $[\![.]\!]^b$ send green spiders, wires, empty diagram, \triangle and λ -boxes to 1, and act differently on red spiders and hadamards. For general x, y, define $[\![.]\!]^{b_{x,y}}$ by:



So we have a list of 16 functors $[\![.]\!]^{b}$, $[\![.]\!]^{b_{i,i}}$, $[\![.]\!]^{b_{-i,i}}$, $[\![.]\!]^{b_{-i,-i}}$, $[\![.]\!]^{b_{i,-1}}$, $[\![.]\!]^{b_{-i,-1}}$, $[\![.]\!]^{b_{-1,-i}}$, $[\![.]\!]^{b_{-1,-i}}$, $[\![.]\!]^{b_{-1,-i}}$, $[\![.]\!]^{b_{-1,-i}}$, $[\![.]\!]^{b_{-1,-i}}$, $[\![.]\!]^{b_{1,-i}}$, $[\![.]\!]^{b$

 $[\![.]\!]^{b_{i,i}}$ and $[\![.]\!]^{b_{-i,-i}}$ do not satisfy: H2, TR6, TR9, IV. $[\![.]\!]^{b_{-i,i}}$ does not satisfy: H2, EU, TR6, IV, and in addition H unless n + m is even (same as $[\![.]\!]^{b}$). $[\![.]\!]^{b_{i,-1}}$ and $[\![.]\!]^{b_{-i,-1}}$ do not satisfy: EU, TR6, TR9, IV, and in addition H unless n+m is a multiple of 4. $[\![.]\!]^{b_{-1,i}}$ and $[\![.]\!]^{b_{-1,-i}}$ do not satisfy: H2, EU, TR9, IV, and in addition H unless n + m is a multiple of 4. $[\![.]\!]^{b_{-1,-1}}$ does not satisfy: IV. $[\![.]\!]^{b_{i,1}}$ and $[\![.]\!]^{b_{-i,1}}$ do not satisfy: EU, TR6, TR9, IV and in addition H unless n + m is a multiple of 4. $[\![.]\!]^{b_{1,i}}$ and $[\![.]\!]^{b_{1,-i}}$ do not satisfy: H2, EU, TR9, and in addition H unless n + m is a multiple of 4. $[\![.]\!]^{b_{1,-i}}$ do not satisfy: H2, EU, TR9, and in addition H unless n + m is a multiple of 4. $[\![.]\!]^{b_{-1,-1}}$ do not satisfy: EU, TR9, IV and in addition H unless n + m is even. $[\![.]\!]^{b_{1,-1}}$ do not satisfy: EU, TR9, IV and in addition H unless n + m is even. $[\![.]\!]^{b_{1,-1}}$ do not satisfy: EU, TR9 and in addition H unless n + m is even. $[\![.]\!]^{b_{1,-1}}$ is simply the standard interpretation. Most of them do not satisfy IV, which is already proven to be necessary, so no new immediate conclusion. The exceptions are $[\![.]\!]^{b_{1,-1}}$, $[\![.]\!]^{b_{1,i}}$ and $[\![.]\!]^{b_{1,-i}}$, however they involves H, which is also shown to be necessary.

The only two triangle rules not satisfied by the above interpretations are TR6 and TR9. We could have define the interpretations on triangle differently to try satisfy the axioms. However, TR9 has two triangles on both sides, and hence such approach will not work. For TR6, setting interpretation on \triangle to be -1 will satisfy the axioms. However axioms TR2, TR3 and AD will now appear as unsatisfied. Hence there is no strictly more refined result that we can produce immediately. Clearly, changing the interpretation on λ will only provide more unsatisfied axioms.

An improvement can be made if we have an alternative IV axiom.

Lemma 4.2.3. If an alternative IV axiom has sum of degrees of red nodes plus number of hadamards equalling multiples of 4, then we can conclude at least one of H2, TR6, TR9 is necessary. Hence, if one of them is derivable, then either of the remaining two has to appear in its proof.

Proof. This follows from the interpretation $[\![.]]^{b_{i,i}}$.

This indicates towards the necessity of the three axioms, since their conceptual meanings are expressing different properties.

In [25], functor $[\![.]\!]^{\bullet}$ is defined that gives the parity of number of odd red nodes plus number of hadamards, and used it to show that a version of empty rule for $\pi/2$ is needed.

Definition 4.2.4. Define $[\![.]\!]^{\bullet}$ as $[\![D_1 \otimes D_2]\!]^{\bullet} = [\![D_1 \circ D_2]\!]^{\bullet} = [\![D_1]\!]^{\bullet} + [\![D_2]\!]^{\bullet}$ mod 2, and $[\![.]\!]^{\bullet} = 0$ for all generators except:



Indeed it turns out that $[\![.]\!]^{\bullet}$ is essentially the same as the $[\![.]\!]^{b_{-1,1}}$ we have above, proving the necessity of IV again.

To develop the parity interpretations further, we modify interpretations on green spider. Define $[\![.]]^{b'_{x,y}}$ to be the same as $[\![.]]^{b_{x,y}}$ for all generators except green spider, and define



We consider what $[\![.]]^{b'_{x,y}}$ adds to the underlying $[\![.]]^{b_{x,y}}$. H now multiplies an extra $(-1)^{n+m}$ on the right, EU has -1 on the right, TR9 has -1 on the right, IV has -1 on the left. Combining with the results above, they give different sets of independence axioms, but the sizes of the sets are not reduced.

So we have completely explored parity-based models and the immediate necessity results they can provide are limited. This is because, unlike in $\pi/2$ -fragment where there is only red, green and hadamard generators, the additional \triangle axioms make parity relationships between generators significantly more complicated, and hence the motivation no longer works well. Intuitively, if we want to follow this line of approach, we need to find an interpretation that express some 'generalised parity relationship' like: when red spiders are turned into green ones, hadamards arise on every leg and \triangle arise at some specific places. From our understanding, this kind of generalised parity relationship does not seem to hold, and it will require significant insights and experiments to discover any.

4.3 $ZX_{\pi/4}$ models

Next we consider interpretations into the category $\mathbf{ZX}_{\pi/4}$, and hence the functors are endofunctors. The similar approach in set theory is constructing inner models, which is widely studied.

Lemma 4.3.1. AD is necessary.

Proof. Define (a set of interpretations) $\llbracket.\rrbracket_n$, as done in [17], by multiplying the angles of red and green phases by n, taking mod 2π . Define $\llbracket.\rrbracket_n$ for \triangle and λ as the same as standard interpretation.



For any n, all standard rules in Figure 2.1, apart from EU and K2, hold, since they are either for general phases, or do not involve phase at all. For the same reason, all lambda rules in Figure 2.3, apart from IV and AD hold. When n is odd, additionally K2 holds, and all triangles rules in Figure 2 holds, since only π occurs as fixed angle for red/green phases, and odd multiples of π under modulo 2π is unchanged. When n=7, we make IV holds, since



This is also the smallest n for it to satisfy IV. However, EU and AD are not satisfied. If we set n=9, then since $\frac{9\pi}{4} \mod 2\pi = \frac{\pi}{4}$ and $\frac{-9\pi}{4} \mod 2\pi = \frac{-\pi}{4}$, IV is again satisfied. In addition, since $\frac{9\pi}{2} \mod 2\pi = \frac{\pi}{2}$ and $\frac{-9\pi}{2} \mod 2\pi = \frac{\pi}{4}$.

 $\frac{-\pi}{2}$, EU is satisfied. AD is still not satisfied since a general instance of AD, giving $\lambda e^{i\gamma} = \lambda_1 e^{i\alpha} + \lambda_2 e^{i\beta}$, does not imply $\lambda e^{9i\gamma} = \lambda_1 e^{9i\alpha} + \lambda_2 e^{9i\beta}$. Therefore AD is necessary.

Note $[\![.]\!]_n$ is used in [17] to prove the necessity of a version of EU for $\pi/2$ -fragment. The argument no longer works, as it is clear from the proof above that any interpretation that does not satisfy EU will not satisfy AD too. Also note that if we use EU' given in Lemma 3.1.5 instead of EU, the proof still works.

Intuitively, AD is the only rule that is not satisfied by the interpretation because it is the only "exponentiation" rule. That is, relationship between angles are not expressible with only addition and multiplication. With this understanding, we give another simpler proof that AD is necessary. The proof is simpler because we exploit the "nonlinearity" in λ , and generator λ occurs in far fewer rules than green and red spiders.

Definition 4.3.2. Define interpretation $[\![.]\!]_{\lambda=1}$, which sends λ to $\lambda = 1$, and is the same as the standard interpretation on everything else.

We can consider how this interpretation act on the rules. Clearly the only rules that might not be satisfied are ones involving λ . L1, L2, L3, L4, L5, TR14 are clearly satisfied. For AD, if $\lambda e^{i\gamma} = \lambda_1 e^{i\alpha} + \lambda_2 e^{i\beta}$, it does not imply in general that $e^{i\gamma} = e^{i\alpha} + e^{i\beta}$. Therefore AD is the only rule not satisfied by $[\![.]\!]_{\lambda=1}$, hence it is necessary.

Definition 4.3.3. Define functor $[\![.]\!]^{\natural}$ for $\pi/2$ -fragment as



The functor $[\![.]\!]^{\ddagger}$ was given in [4] to show necessary of scalar ZO rule in $\pi/2$ -fragment. We need to extend to $\pi/4$ -fragment by adding interpretations for $\pi/4$ -phases, \triangle and λ .

We motivate the reason behind our extension. We think $\pi/4$ spiders should be something "in between" 0 and $\pi/2$ ones. Consider green node with one input and one output, if phase is 0 or π , its \natural -interpretation is double wire. If phase is $\pi/2$ or $-\pi/2$, it's CNOT gate, because we have:

	п	<i>`</i> 1	0	0	$0 \setminus$
	_↓∥ _	0	1	0	0
		0	0	0	1
Ш	Ш	0	0	1	0/

Therefore, we want to find the square root of CNOT.

Lemma 4.3.4. One square root of CNOT is





This coincidentally terms out to correspond to the simple matrix square root too.

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1/2(1+i) & 1/2(1-i) \\ 0 & 0 & 1/2(1-i) & 1/2(1+i) \end{pmatrix}$$

Then we generalise the square root to arbitrary number of inputs and outputs. This gives our definition for $\pi/4$ -phases. For \triangle , it is easy to see that doubling will not work. Therefore, we calculate the decomposition of \triangle in $\pi/4$ -phases, as given in Lemma 3.3.2, under $[\![.]\!]^{\natural}$. We hence reach our definition.

Definition 4.3.5. Extend the $\llbracket . \rrbracket^{\natural}$ to $\pi/4$ -fragments, by defining it on $\pi/4$ -spiders, \triangle and λ .



Consider the axioms under the interpretation. From [4], we already know that all rules in Figure 2.1, when restricted to $\pi/2$ -fragment, holds. So it remains to check the $\pi/4$ -multiple phases for S1, H and K2. S1 is satisfied just by Lemma 4.3.4. H is satisfied just by application of H2. For K2 with $\alpha = \pm \frac{\pi}{4}, \pm \frac{3\pi}{4}$, equality of the K2 under [].]^{\u03c4} reduces to verifying the equality of the following constant,



, which holds, by completeness, since they calculate that both are $\sqrt{2}$ under the standard interpretation. So all rules in Figure 1 are satisfied. IV is also satisfied by using Lemma 3.1.3 in the calculation.

Next is to verify whether the \triangle and λ rules hold. The interpretation of \triangle is very complicated and does not seem to simplify. Its corresponding

matrix is

So it's easy to see few triangles rules are satisfied by $[\![.]\!]^{\natural}$. However if we assume the sqrt-CNOT gate can slide through spiders, the triangle interpretation becomes:



This interpretation of triangle is a lot simpler. Consider the triangle axioms under this new interpretation.

Lemma 4.3.6. At least one of TR2, TR9, TR13, AD is necessary.

Proof. Axioms not satisfied by $[\![.]\!]^{\natural}$ are TR2, TR4', TR9, TR10', TR13, AD. TR4' and TR10' are derivable. Under $[\![.]\!]^{\natural}$, TR5, TR6 are satisfied, up to a constant, which can be ignored.

Remark 4.3.7. Constants can be ignored since we can modify the definition of equality, and define diagrams to be equal if they are equal up to a constant. Hence the functor is no longer from $\mathbf{ZX}_{\pi/4}$ to $\mathbf{ZX}_{\pi/4}$, but rather to a modified $\mathbf{ZX}'_{\pi/4}$.

Changing the interpretation of λ to 0 (absorbing constant), rather than double wire, we can change the result to: At least one of TR2, TR9, TR13, L3 is necessary. But neither gives immediate necessity result, since AD and L3 are known to be necessary. This still strongly suggest the necessity of TR2, TR9, TR13, since they are expressing different meanings.

Remark 4.3.8. Note that the simplification of the interpretation of \triangle we carried out is not a formal derivation, i.e. the equation is not true in $\mathbf{ZX}_{\pi/4}$, and sqrt-CNOT does not 'slide' pass spiders. But this is exactly why the above set of axioms get picked out (i.e. not satisfied). We are using a 'slightly wrong' equation, and this tells us which axioms will be 'wrong' under the interpretation. If one can come up with a definition that is 'less wrong' than the one we give, then it is likely that they can prove the necessity of one of those axioms (TR2, TR9 or TR13).

Next consider another interpretation into $\mathbf{ZX}_{\pi/4}$.

Functor $[\![.]\!]^{\sharp}$ is given in [33] to establish the necessity of a supplementarity rule for $\pi/2$ -fragment, we extend it to $\pi/4$ -fragment.

Definition 4.3.9. Define $[\![.]\!]^{\sharp}$ the same on red, green and hadamard, tripling and adding a gadget that doubles the angle, and a scalar dot at the side. Extend it to include \triangle and λ .



Lemma 4.3.10. At least one of TR13, IV, AD is necessary.

Proof. The interpretation $[\![.]\!]^{\sharp}$ is sound for all rules apart from TR13, IV, AD, L5. L5 is derivable. For rules involving angles that are only 0, π , it's clear, by simplifying the gadget using B1 rule twice. For some with general

angles or $\pi/2$, $\pi/4$, such as S1, K2, H, it has been shown in [33]. Intuitively the above four fail because when the angles involved are not multiples of $\pi/2$, the gadgets often do not simplify in this case.

In a remark in [33] it is pointed out that $\llbracket.\rrbracket^{\sharp}$ can be extended to $\llbracket.\rrbracket_{k,l}^{\sharp}$ where k is the number of copies and l is the multiplication coefficient of the gadget's phase, with k-1 constant dots. So the one given above is $\llbracket.\rrbracket_{3,2}^{\sharp}$.

So we can do better, by considering $[\![.]]_{3,8}^{\sharp}$. It in addition satisfies the IV rule, since $\pi/4 \times 8 = 2\pi$, and the gadget disappears. So we can conclude that either AD or TR13 is necessary. Although we have already showed AD is necessary, this result still gives strong indication that TR13 is indeed necessary. If it is derivable, AD must be used in its derivation, which we think is very unlikely.

Remark 4.3.11. Throughout the chapter, we stated many axioms have different meanings. This informal statement can be understood in mainly two ways. One is their structural meanings. Using TR1 and TR2 as examples, we can think of TR1 as saying a commutation relationship between red π and Δ , and TR2 saying ' Δ does nothing on a red state'. Second is the information they express about corresponding matrices under [[.]]. If we assume,

$$\left[\begin{array}{c} \checkmark \\ \hline \\ \hline \\ \hline \\ \end{array} \right] = \begin{pmatrix} a & b \\ c & d \end{pmatrix},$$

then TR1 is saying a = d, and TR2 is saying a = 1, c = 0. One might want to take this approach further, by changing matrix interpretations in **FHilb**, to prove independence, but attempts show that such functors into **FHilb** are not expressive enough to distinguish many axioms.

To sum up, we have proved necessity of S1, H, IV, S3, L3, AD. There are also some weaker independence results that hint at the possible necessity of H2, B1, TR2, TR5', TR6, TR9, TR13.

Chapter 5

Alternative presentations of axioms

In this section we consider alternative presentations of ZX-calculus. Different presentations will be useful for different purposes, and the definitions of axioms are often a design decision. Indeed, the $\mathbf{ZX}_{\pi/4}$ axioms we use, from NW paper, contain 30 small axioms (before simplification) with 5 symbols: red, green, hadamard, triangle, lambda. In the JPV paper, there is only 12 axioms, with 3 symbols: red, green, hadamard. However, the largest axiom has 21 nodes in it. This is already reduced from the version 1 of the paper, which had axioms C1, C2, C3 that have 18, 20 and 36 nodes respectively.

Apart from the trade-off between quantity and sizes of axioms, another main advantage of the NW paper, as they pointed out, is the natural occurrence of \triangle in the diagrammatic form of Toffoli gate. This is one of the elementary component of quantum circuits, and it's decomposition in standard quantum circuit literature, in terms of other unitaries and CNOT, is a lot more complicated.

In some sense, the NW axioms achieves theoretical purpose and practical convenience at the same time, at the expense of more generators and axioms. As an analogy in logic, we are interested in finding a minimal and adequate set of primitive connectives, for example $\{\neg, \rightarrow\}$ or simply one binary connective $\{\uparrow\}$, but also in have a natural and useful set, for example \land, \lor, \neg .

It should appear that λ and green spider are indeed very similar generators, as also noted in [30], and a notion of generalised spider is defined. In [13], such generalised spider is used in simplifying quantum circuits. It should be evident for many reasons that λ and green spider can be combined. All the lambda rules (except AD), when putting green nodes with certain phases in place of the λ boxes, hold. As pointed out, TR13 and TR14can be merged into one. This is because λ and green spider are essentially describing the two parameters of a complex number $\lambda e^{i\alpha}$.

Definition 5.0.1. Define new generator with its standard interpretation,

		_		2^n			
	ſ	$\left(\begin{array}{c} 1\\ 0\\ . \end{array} \right)$	0 0		0 0	$\begin{pmatrix} 0 \\ 0 \\ \cdot \end{pmatrix}$	
	$:= 2^m \left\{ $	$ \begin{bmatrix} \vdots \\ 0 \\ 0 \end{bmatrix} $: 0 0	· · · ·	: 0 0	$\begin{array}{c} & \\ & 0 \\ \lambda e^{i\alpha} \end{array}$,

where $\lambda \in \mathbb{Z}[\frac{1}{2}], \alpha \in \{\frac{k\pi}{4} | k = 0, 1, \dots, 7\}.$

The original set of axioms is still sound and complete with the change of notation:



To exploit the notational convenience, we change axiom S1 into GS1,



The instances of $\lambda_1 = \lambda_2 = 1$ gives the original S1. Hence this set of axiom is still sound and complete. However, the λ axioms" are significantly reduced.

Lemma 5.0.2. L1, L3, L4, L5 are all derivable.

Proof. L1, L4, L5 are just instances of GS1. L3 is just S2.

Additionally, AD and TR13' now becomes:



Note that all the necessity results existing axioms still remain, plus GS1 being necessary (follows from the same argument as the necessity of S1).

The proposed generalised spider node in [30] has one parameter, a, which takes value of any complex number, and is used for unrestricted ZX-calculus. Since we would like to work within the $\pi/4$ -fragment, using two parameters for polar coordinate is more convenient.

Another possible simplification is to make the rules having a smaller number of nodes. For example, we can consider defining a new generator for a commonly occurring subdiagram.

Definition 5.0.3. Define new generator white triangle and its standard interpretation as,

$$\begin{vmatrix} & & \\ &$$

and add one axiom W1:



W stands for either white triangle or W-state. Indeed this component has matrix which is the almost the same as the black dot generator (the W-state) for ZW-calculus. In the recent version 2 of [24], they also pointed this out in the proof of completeness, as an abbreviation in the lemmas. We take a step further and use it as a generator in the axioms since it seems to appear as a primitive component.

The exact correspondence between black dot in ZW and ZX is:



We choose to use a new symbol, rather than the black dot, since at this stage we do not want to mix up symbols of ZW and ZX calculus yet, as

it can be confusing, unless there is more evidence to suggest this should happen. $\mathbf{ZX}_{\pi/4}$ with the new generator and added axiom W1 is still sound and complete.

AD becomes much more intuitive:



Therefore we can use a simpler axiom, maintaining soundness and completeness.



So it turns out that the white triangle is exactly the "addition device"

Many other triangle rules can be immediately simplified with the new generator, in particular, TR7, TR8, TR9, TR13. Again note that the previous necessity results still hold.

Chapter 6

Conclusion and future work

6.1 Conclusion

To sum up, we have derived S2, TR3, L2, L5, simplified K2, TR13, TR14, L4 and changes EU to a simpler EU'. We showed S1, S3, H, IV', AD, L3 are necessary. In particular AD, which is the only 'nonlinear' axiom that relate λ and phases by an exponential equation in the metatheory.

We proved that any three axioms among H2, H, EU, TR6, TR9, together with IV, is independent from the rest, using parity-based interpretations. We proved that at least one of TR2, TR9, TR13, together with either AD or L3, is independent, and then a stronger result (proved using a completely different interpretation) that either TR13 and AD is necessary. They point to the likelihood of the necessity of the axioms, which is indeed helpful, since when one is presented with an axiom, they have to decide whether they should attempt to derive it or prove independence first, by some informed guessing. It is potentially possible to use these independence results in conjunction with new results one discover, to show necessity.

The results have more implications. Firstly, the lambda rules are indeed understood very well now. The only remaining ones are AD, L3, L4 and TR14, with AD and L3 shown to be necessary. We then presented the generalised spider rule that removes λ as a separate generator, and backed up the proposal by pointing out the structural similarities between green spiders and λ . Secondly, after the removal of the derivable Δ rules, we pointed out the frequent occurrences of W-states in the remaining Δ rules, and proposed the possibility of taking it as a primitive generator.

The interpretations we extended not only prove independence results, but also allow us to understand the meanings of the axioms and how they are used. In some sense, they can be seem as approximate models of $\mathbf{ZX}_{\pi/4}$.

We present the new set of axioms, removing the derivable ones, and adopt the two presentations we gave, in Figure 6.1, 6.2.



Figure 6.1: The updated standard ZX rules for $\pi/4$ -fragment. $\alpha, \beta \in \{\frac{k\pi}{4} | k = 0, 1, \dots, 7\}, \lambda \in \mathbb{Z}_{\frac{1}{2}}^{\frac{1}{2}}$.



Figure 6.2: The updated triangle rules for $\pi/4$ -fragment. In AD', $\lambda_1 e^{i\alpha} + \lambda_2 e^{i\beta} = \lambda e^{i\gamma}$. In TR13", $\lambda = \frac{1}{2}$ or $\lambda = p$, p prime.

6.2 Future work

The study of axioms of ZX-calculus, and ZX-calculus in general, is far from finished, we give some potential directions for future developments in a few different areas. Regarding independence and necessity of axioms:

- Axiom L4: On the one hand, we think it should be derivable, since it seems be possible to define multiplication in terms of addition, rather than taking it as a primitive, for λ. On the other hand, attempts reduce the axiom to some equation between △ that do not seem to simplify. L4 also appears as an instance of a necessary axiom GS1, using the alternative presentation. This is the only axiom for which we are very unsure about its necessity and it is worth investigating further.
- 2. Consider modifications of our interpretations into $\mathbf{ZX}_{\pi/4}$. In particular, changing the definition of \triangle in $[].]^{\natural}$. There is a possibility that with some clever construction this approach can prove the necessity of TR2 or TR9 or TR13.
- 3. Consider other new interpretations into $\mathbf{ZX}_{\pi/4}$. The types of interpretations we have are in general, multiplying phases and making approximate copies of the diagrams. There are clearly other types of constructions.
- 4. Consider interpretations into other specific categories. They should all be \dagger -CCC, since examples of other categories will simply satisfy very few axioms. Suggestions we have are finite relations **FRel**, **Spek** which is a subcategory of **FRel** [10] and the category of 2D corbodisms **2Cob** [12]. The difficulty in mapping into **FRel** (or **Spek**) is the definition of \triangle again. We have not attempted to map into **2Cob**. Indeed, **2Cob** is the domain of the subject of topological quantum field theory, and if a functor from $\mathbf{ZX}_{\pi/4}$ into **2Cob** which satisfies the majority of the axioms exist, it will be surprising and indeed have a lot more implications beyond independence.
- 5. Apply our interpretations for axioms in the JPV paper [24]. Since their axioms do not involve \triangle and λ , proofs of necessity will be easier. Many of our results about the standard rules (which appear in the JPV set of axioms) should already carry over.
- 6. Borrow other independence proof techniques from model theory or set theory, for example the common method of forcing for sets. The major difficulty is that the theory (and metatheory) we are working in is completely different. Even our symbols and syntax are different (which is the whole point of ZX-calculus), as their geometry encodes

information. Hence, one needs to design analogies of exisiting techniques which is the main difficulty.

- 7. Investigate the remaining open questions about necessity in $\pi/2$ -fragment. A main open axioms is B2, which also appears in our standard rules, and is left open again. It is generally believe that B2 (the bialgebra rule) is necessary.
- 8. Simplify and investigate necessity of axioms of general pure qubits quantum mechanics (i.e. full ZX-calculus) in [29]. This task is even harder than for the $\pi/4$ -fragment, since having the uncountable set of angles and λ ranging over all non-negative \mathbb{R} means that none of our definitions can be easily carried over.

We then give a few general open questions for $\pi/4$ -fragment of ZX-calculus:

- 1. The decomposition of \triangle in Lemma 3.3.2 is correct, by matrix calculations and completeness theorem. However, there is no known derivation of the decomposition within $\mathbf{ZX}_{\pi/4}$. That means we don't know what axioms are needed in obtaining the decomposition. Having an internal derivation is helpful both in understanding \triangle better, and in potentially derive other \triangle axioms.
- 2. Investigate alternative simpler presentations, and whether the white triangle symbol (W-state) should be used as a primitive. This can also be generalised to a question of investigating the relationships between ZW and ZX-calculus.

The target is to aim to have sets of axioms for π , $\pi/2$ and $\pi/4$ -fragments of ZX-calculus, each extending the previous ones, and are also minimal. At the moment each fragment has their own unique axioms and have open questions about necessity.

We also give a few further directions to the development of ZX-calculus in other areas:

- 1. Consider the applications of ZX-calculus, in particular, in the simplification of quantum circuits. [13] used a different set of rules for 2-qubit Clifford+T quantum circuits (with a different notion of completeness). It will be useful to try find a set of axioms, possibly modify ours, so that they are axioms which achieve theoretical completeness, and 'axioms of circuits', at the same time.
- 2. Investigate other applications of ZX-calculus. For example, the use of ZX-calculus in quantum error correction [8], [14]. More recent work by Quanlong Wang that is not yet published shows that we can do linear algebra using ZX. This immediately opens up many other related possibilities.

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