Addition and Differentiation of ZX-Diagrams

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Abstract

The ZX-calculus is a powerful framework for reasoning in quantum computing. It provides in particular a compact representation of matrices of interests. A peculiar property of the ZX-calculus is the absence of a formal sum allowing the linear combinations of arbitrary ZX-diagrams. The universality of the formalism guarantees however that for any two ZX-diagrams, the sum of their interpretations can be represented by a ZX-diagram. We introduce a general, inductive definition of the addition of ZX-diagrams, relying on the construction of controlled diagrams. Based on this addition technique, we provide an inductive differentiation of ZX-diagrams.

Indeed, given a ZX-diagram with variables in the description of its angles, one can differentiate the diagram according to one of these variables. Differentiation is ubiquitous in quantum mechanics and quantum computing (e.g. for solving optimization problems). Technically, differentiation of ZX-diagrams is strongly related to summation as witnessed by the product rules.

We also introduce an alternative, non inductive, differentiation technique rather based on the isolation of the variables. Finally, we apply our results to deduce a diagram for an Ising Hamiltonian.

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1 Introduction

The ZX-calculus is a graphical language for manipulating linear maps. It was originally introduced in [4] and proven to be complete for qubit quantum computation [13, 11, 16, 25]. A general introduction to the language alongside the overview of the main applications is available in [24].

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Due to its flexibility, ZX-calculus became widely used to address different problems of quantum computing. However, its application to the rapidly growing field of variational algorithms [3] like QAOA [7] *(quantum approximation optimization algorithm)* and VQE [20] (*variational quantum eigensolver*) are so far limited. Nevertheless as variational algorithms do not require heavy resource for error-correction, the incoming emergence of *NISQ* devices makes from them an object of particular attention [21]. We believe that the reason why they are still unexplored with the means of ZX-calculus is the absence of a convenient way to differentiate parametrized diagrams. Indeed, basic building blocks of variational algorithms are parametrized circuits and the search of optimal parameter values is a crucial part of these algorithms. The search is usually done by classical numerical optimization methods [8] and most of them use derivatives.

The main difficulty for differentiation of ZX-diagrams comes from the *product rules* that involve sums. Several attempts were made to face this problem [29, 23]. The paper [23] extends the signature of ZX-category to formal sums of diagrams while [29] provides explicit derivatives for diagrams with the number of parameter occurrences limited to two. The first option that is to use formal sums has major disadvantages as there is no rules to manipulate sums of ZX-diagrams.

In our approach the derivative of a parametrized ZX-diagram is another ZX-diagram. Hence we avoid the extension of the signature with formal sums. In order to tackle sums that appear in the product rule, we introduce an original technique to perform the addition of diagrams entirely in the ZX-calculus. We use special diagrams called controlled states [15]. We suggest a way to represent every ZX-diagram by such a state. As we know how to sum controlled states [15] the addition for arbitrary diagrams follows. An inductive definition of the derivative is obtained by explicit diagrammatic representation of the product rules.

Very recently an independent work with a similar result, although obtained from a different approach, was published on *arXiv* [27]. In contrast to our work, the authors of [27] use algebraic ZX-calculus [26] and W-spiders [10] to express derivatives. Their paper highlights the crucial role that W-spider plays in the representation of sums. However, it does not provide an algorithm of diagrammatic addition for arbitrary diagrams.

In an attempt to give a ready-to-use toolbox for differentiation, we provide an easy and convenient way to compute the derivative for the family of linear diagrams ZX(β) [15]. Most of circuits for variational algorithms belong to ZX(β) and we believe that our formulas will make the analysis of them much simpler.

In the end, we show how our result together with the Stone's theorem [22] allows to find a ZX-diagram for an Ising Hamiltonian - another key component of variational quantum algorithms [9].

Structure of the paper

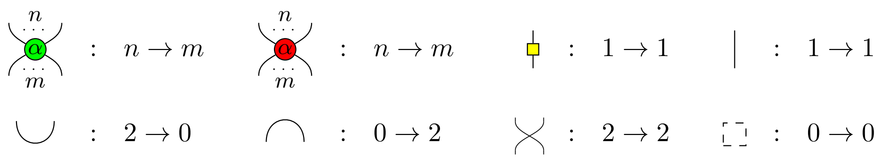
In the section 2, we give a brief introduction to the ZX-calculus. In the section 3, we recall the properties of controlled states and give the definition of *controlizer*: a map that transforms an arbitrary diagram to a controlled state. We show how to use controlizers to perform the addition of ZX-diagrams. In the section 4, we introduce the formal semantics of derivative of a parametrized diagram. The definition is followed by an algorithm for differentiation that explicitly incorporates the product rule. Finally, we give two compact formulas for derivatives in ZX(β) that may be directly used in computation. In the section 5, we show how to apply our result to obtain a diagram for an Ising Hamiltonian. Most of proofs are detailed in the full version of our paper that is available online [12].

2 ZX-calculus

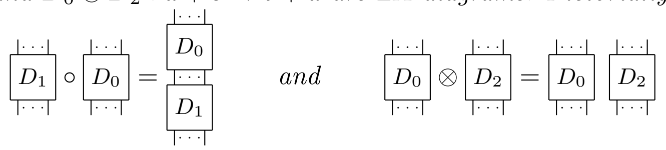
2.1 Syntax and Semantics

The ZX-diagrams are generated by green spiders , red spiders and Hadamard , where both kinds of spiders have an arbitrary number of inputs/outputs and are decorated with angles. ZX-diagrams are also made of wires: the identity , the swap and also the possibility to bend wires with a cup and a cap . Finally, the empty diagram is denoted .

▶ **Definition 1.** ZX-*diagrams are inductively defined as follows: for* $n, m \in \mathbb{N}$ *and* $\alpha \in \mathbb{R}/2\pi\mathbb{Z}$,



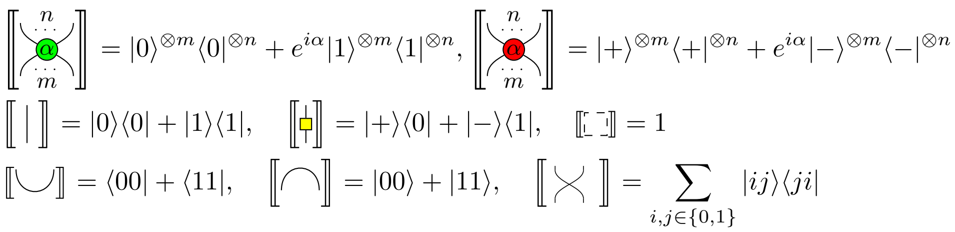
are ZX-*diagrams, and for any* ZX-*diagrams* $D_0 : a \to b$, $D_1 : b \to c$, *and* $D_2 : c \to d$, $D_1 \circ D_0 : a \to c$ *and* $D_0 \otimes D_2 : a + c \to b + d$ *are* ZX-*diagrams. Pictorially:*



A diagram with no input/ouput is called a *scalar*. In order to compactly write scalar factors, we introduce syntactic sugar $[-]^{\otimes n}$. For any scalar $d : 0 \to 0$ the notation $d^{\otimes n}$ corresponds to $\underbrace{d \otimes \cdots \otimes d}_{n}$.

Semantically, ZX-diagrams are standardly interpreted as linear maps, and thus they can be used to represent quantum evolutions.

▶ **Definition 2.** *For any* ZX-*diagram* $D : n \to m$, *let* $[\![D]\!] \in \mathcal{M}_{2^m,2^n}(\mathbb{C})$ *be inductively defined as:* $[\![D_1 \circ D_0]\!] = [\![D_1]\!] \circ [\![D_0]\!]$, $[\![D_0 \otimes D_2]\!] = [\![D_0]\!] \otimes [\![D_2]\!]$, *and*



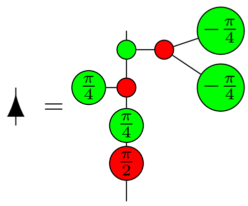
where bra-ket *notations are used:* $|0\rangle = \binom{1}{0}$, $|1\rangle = \binom{0}{1}$, $|+\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$, $|-\rangle = \frac{|0\rangle-|1\rangle}{\sqrt{2}}$, $|xy\rangle = |x\rangle \otimes |y\rangle$ *and* $\langle x| = |x\rangle^\dagger$ *is the adjoint (complex conjugate) of* $|x\rangle$.

Sometimes it is meaningful to consider diagrams with angles from a restricted sub-group $\mathcal{G}$ of $\mathbb{R}/2\pi\mathbb{Z}$. Such restrictions lead to *fragments* of the language, denoted $\text{ZX}_{\mathcal{G}}$-calculus [15]. The standard interpretation associates to each $\text{ZX}_{\mathcal{G}}$-diagram $D : n \to m$ a matrix $[\![D]\!] \in \mathcal{M}_{2^m,2^n}(\mathcal{R}_{\mathcal{G}})$ with elements in the ring $\mathcal{R}_{\mathcal{G}} = \mathbb{Z}\left[\frac{1}{\sqrt{2}}, e^{i\mathcal{G}}\right]$ - the smallest ring that contains $\mathbb{Z}$, $\frac{1}{\sqrt{2}}$ and $\{e^{ia} | a \in \mathcal{G}\}$ [15].

In particular the $\frac{\pi}{2}$- (resp. π-) fragment[1], also called Clifford (resp. real Clifford) fragment, enjoys nice properties [1, 6] but is not universal for quantum computing, even approximately. Furthermore any quantum computation that can be expressed in this fragment can be efficiently simulated on a classical computer. As soon as the group contains the angle $\frac{\pi}{4}$, the corresponding fragment is approximatively universal for quantum computing: any $2^n \times 2^n$ unitary transformation can be approximated by a ZX-diagram from this fragment with arbitrary precision. In particular the $\frac{\pi}{4}$-fragment, also called "Clifford+T" fragment has been extensively studied [13, 17, 19]. Other finitely generated fragments have been considered in [15].

Notice that for any sub-group $\mathcal{G}$ of $\mathbb{R}/2\pi\mathbb{Z}$ that contains $\frac{\pi}{4}$, $\mathrm{ZX}_\mathcal{G}$-diagrams are *universal* [15] in the sense that for any matrix $M \in \mathcal{M}_{2^m,2^n}(\mathcal{R}_\mathcal{G})$ there exists a $\mathrm{ZX}_\mathcal{G}$-diagram $D : n \to m$ such that $[\![D]\!] = M$.

In this work we extensively use triangle:  - a syntactic sugar introduced in [13]. It corresponds to a non-unitary transformation: $[\![$  $]\!] = |0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 1|$. The triangle may be written in terms of red and green spiders as:

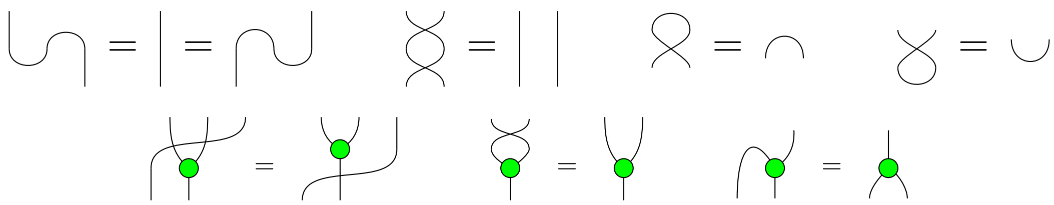


(1)

2.2 The calculus

Two ZX-diagrams may have the same interpretation, as a consequence the language is equipped with a set of rewrite rules (Figure 1) that allows to transform diagrams.

In addition, ZX-diagrams can be deformed at will: all wires may be bent in any manner that keeps intact the order of inputs and outputs. It is also allowed to arbitrary change the order of wires for green and red spiders and the Hadamard. Corresponding transformation rules are aggregated under the paradigm *Only topology matters*:



We denote $\mathrm{ZX} \vdash D_1 = D_2$ if D_1 may be transformed to D_2 by local application of rewriting rules.

The ZX-calculus is sound, i.e. the rules preserve the semantics: if $\mathrm{ZX} \vdash D_1 = D_2$ then $[\![D_1]\!] = [\![D_2]\!]$. The converse property is called completeness. The set of rules (1) was proven complete for the $\frac{\pi}{4}$-fragment [15], and a single extra-rule makes the language complete for arbitrary diagrams [14]. Notice that alternative sets of rules have been shown to be complete for general ZX-diagrams [11, 25]. We choose to consider the rules of Figure 1 as they have been used to study diagrams with parameters in [14], which is an appropriate framework for differentiation (see section 4).

[1] I.e. the fragment of diagrams which angles are in the group generated by $\frac{\pi}{2}$ (resp. π)

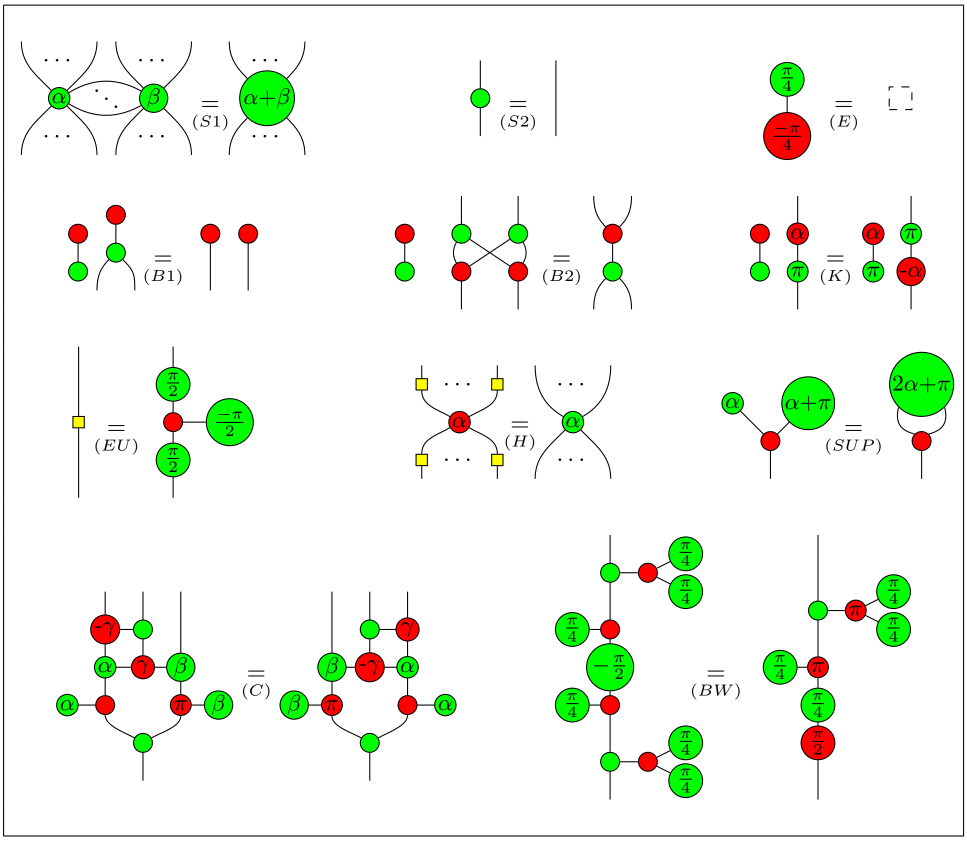
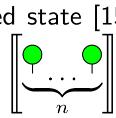


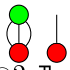
Figure 1 Axioms for ZX as presented in [15]. All rules stay true flipped upside down and with inverted colors. Families of equations are given using "dots": ... means any number of wires, ⋱ means at least one wire.

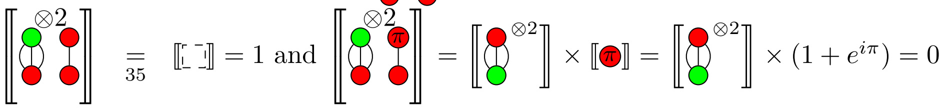
3 Addition of ZX-diagrams

The ZX-calculus is a convenient tool for manipulating compositions and tensor products of linear maps. These two operations have natural physical interpretations, corresponding to sequential and parallel compositions respectively. The addition is a natural operation on matrices and it can be interpreted as the superposition phenomenon in quantum mechanics. However, the addition is not a physical process, hence it is not reflected in the standard ZX-calculus [5]. On the other hand, for any two diagrams $D_1, D_2 : n \to m$, the universality of the ZX-calculus guarantees that there exists a diagram $D : n \to m$ such that $[\![D]\!] = [\![D_1]\!] + [\![D_2]\!]$.

We provide in this section a general construction for such a diagram. As pointed out in [15] for the definition of normal forms in the ZX-calculus, one can inductively define the addition on "controlled" versions of the diagrams. A controlled version of a diagram D_0 is roughly speaking a diagram with an extra input such that when this extra input is set to $|1\rangle$ the diagram behaves as D_0 and when it is set to $|0\rangle$ the diagram behaves as a neutral diagram. In order to construct controlled versions, we pass by controlled states:

▶ **Definition 3** (Controlled state [15]). *A ZX-diagram $D : 1 \to n$ is a controlled state if* $[\![D]\!] \, |0\rangle = \sum_{x \in \{0,1\}^n} |x\rangle =$ .

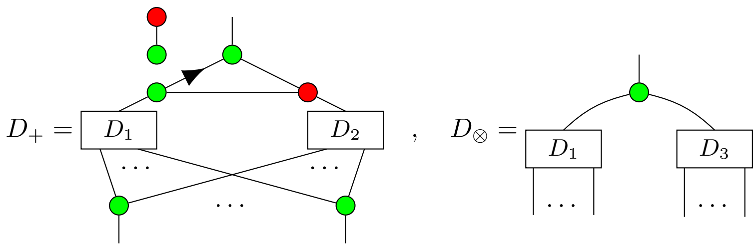
▶ **Example 4.** The diagram  is a controlled state for the scalar 0. Indeed,



Intuitively, a controlled state is a way to encode the state $[\![D]\!]\,|1\rangle$.

Controlled states have nice properties that allows to perform element-wise addition and tensor product of corresponding vectors:

▶ **Lemma 5** (Sum and tensor product [15]). *For any controlled states $D_1, D_2 : 1 \to n$ and $D_3 : 1 \to m$ the diagrams:*



(2)

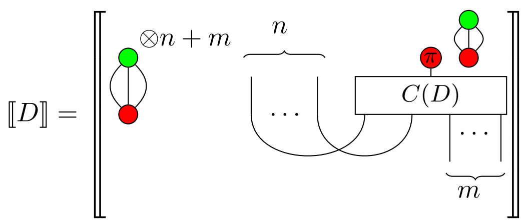
are controlled states, $[\![D_+]\!]\,|1\rangle = [\![D_1]\!]\,|1\rangle + [\![D_2]\!]\,|1\rangle$ *and* $[\![D_\otimes]\!]\,|1\rangle = [\![D_1]\!]\,|1\rangle \otimes [\![D_3]\!]\,|1\rangle$.

Lemma 5 provides a way to obtain a sum of two diagrams in a controlled state form. In order to extend the addition to *arbitrary* diagrams we introduce *controlizers* - maps that associate diagrams with the corresponding controlled states. Formally,

▶ **Definition 6** (Controlizer). *We say that a map $C : \mathrm{ZX}(n, m) \to \mathrm{ZX}(1, n+m)$ that associates to every diagram $D : n \to m$ a diagram $C(D) : 1 \to n + m$ is controlizer if the following conditions hold for any* ZX*-diagram D:*

(i) *$C(D)$ is a controlled state*

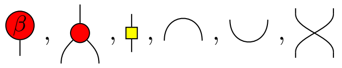
(ii)

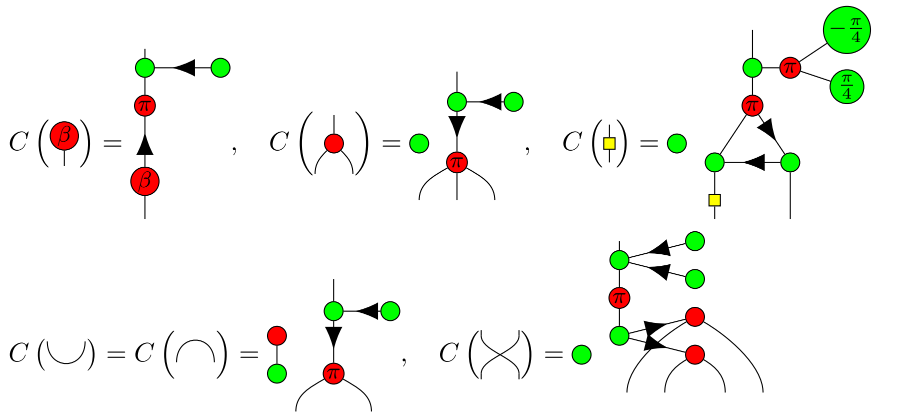


(3)

In this definition (and what follows) $\mathrm{ZX}(n, m)$ denotes the set of ZX-diagrams with n inputs and m outputs. If n and m are not specified, they may take arbitrary values.

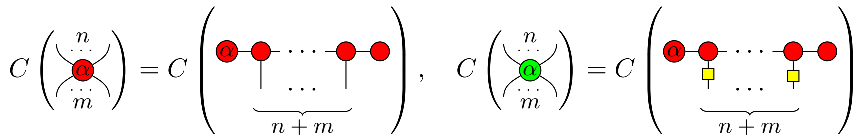
▶ **Example 7** (Inductive controlizer). We define the map $C : \mathrm{ZX}(n, m) \to \mathrm{ZX}(1, n + m)$ that associates to each diagram $D : n \to m$ a diagram $C(D) : 1 \to n + m$:

(i) For the generators :

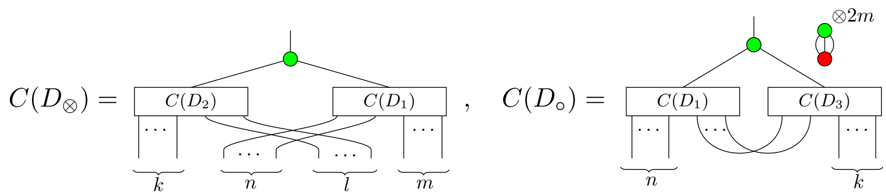


(4)

(ii) Generators  and  can be decomposed as follows using the above generators:



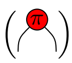
(iii) For tensor product $D_\otimes = D_2 \otimes D_1$ and composition $D_\circ = D_3 \circ D_1$ where $D_1 : n \to m$, $D_2 : k \to l$ and $D_3 : m \to k$:

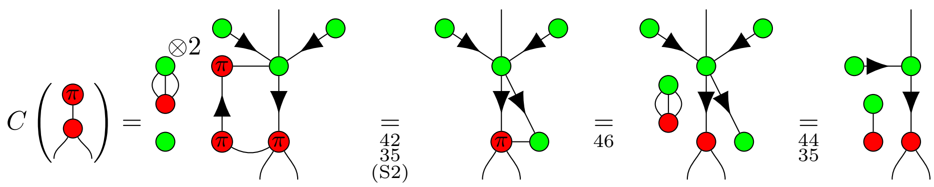


(5)

▶ **Lemma 8.** *The map from Example 7 satisfies the definition of controlizer.*

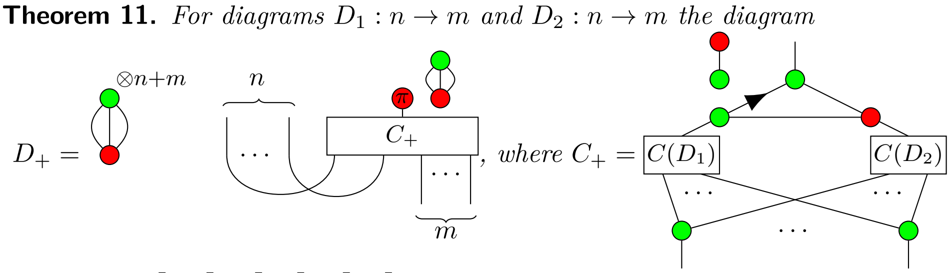
▶ Remark 9. A step-by-step application of the map C may lead to different diagrams depending on the order of decomposition on tensor products and compositions. However, all possible outputs are semantically equivalent and by completeness of ZX-calculus are equivalent as diagrams.

▶ **Example 10.** We show how to obtain C  using definition 7:



(6)

▶ **Theorem 11.** *For diagrams $D_1 : n \to m$ and $D_2 : n \to m$ the diagram*

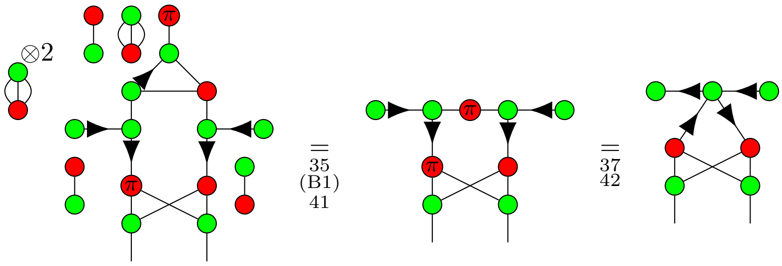


is such that $[\![D_+]\!] = [\![D_1]\!] + [\![D_2]\!]$.

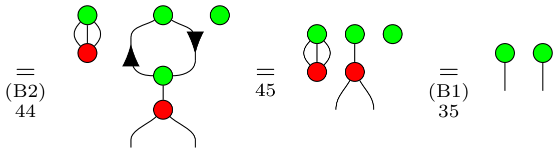
Proof (Theorem 11). The theorem follows from the definition of controlizer and Lemma 5. ◀

We illustrate the diagrammatic addition with a simple example:

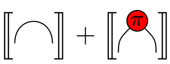
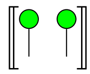
▶ **Example 12.** Using Theorem 11, we construct a diagram D as the addition of  and , which can be simplified as follows, using the rules of the ZX-calculus:

$D =$ 

(7)



(8)

Indeed,  $= (|00\rangle + |11\rangle) + (|01\rangle + |10\rangle) = 2|{+}{+}\rangle =$ .

4 Differentiation of ZX-diagrams

Mathematically, ZX-diagrams form a symmetric monoidal category [4] with natural numbers as objects and diagrams as morphisms. Notice that a definition of the differential category *with respect to morphism's domain* is given in [2]. In the current work, in contrast, we operate parametrized morphisms and derivatives are considered *with respect to parameters*. For example, for the category of matrices with elements that are smooth functions on some variable β we are interested in the derivative over β. We say that a ZX-diagram D is parametrized by $\beta_1, \dots, \beta_k$ if its angles are some functions on $\beta_1, \dots, \beta_k$. We denote such a diagram by $D(\beta_1, \dots, \beta_k)$. [2]

We want to define the formal semantics for the derivative of a parametrized diagram that is consistent with existing definitions of derivatives in monoidal categories with parametrized morphisms.

The work [23] defines the derivative for *monoidal categories with sum* [3] in the following way.

▶ **Definition 13** (Derivative [23])**.** *A derivative $\partial_M : C(x, y) \to C(x, y)$ in a monoidal category M with sum $(+)$ is a sum-preserving unary operator that satisfies the following axioms (product rules):*
$\circ$-product rule: $\partial_M[A \circ B] = \partial_M[A] \circ B + A \circ \partial_M[B]$
$\otimes$-product rule: $\partial_M[A \otimes B] = \partial_M[A] \otimes B + A \otimes \partial_M[B]$

---

[2] We can *evaluate* each parametrized diagram $D(\boldsymbol{\beta})$, $\boldsymbol{\beta} \in \mathbb{R}^k$ in a point $\boldsymbol{\beta}^0 \in \mathbb{R}^k$ by replacing every occurrence of β_i with the respective value β_i^0. The result of evaluation is a diagram $D(\boldsymbol{\beta}_0)$ from $\mathrm{ZX}_{\mathbb{R}}$.

[3] Formally, sum $(+)$ is a commutative monoid that maps each pair of morphisms with same domains/codomains to another morphism. The sum is distributive with respect to composition and tensor product.

Because of the sums involved in product rules, we avoid to directly use the derivative as defined above. Indeed, even if the Theorem 11 provides a fully diagrammatic way for the addition of ZX-diagrams, the formal introduction of a sum monoid leads to unnecessary complications.

On the other hand, for any group $\mathcal{G}$ the category $\mathcal{M}(\mathcal{G})$ of matrices with elements in $\mathcal{G}$ admits a natural definition of sums: the sum $(+_M)$ of two matrices is obtained by entrywise addition. Therefore, we get the semantics of the derivative ∂_M in $\mathcal{M}(\mathcal{G})$ directly from Definition 13. It was proven in [23] that for the category of parametrized linear maps with elements that are smooth functions $S : \mathbb{R}^n \to \mathbb{C}$ an entrywise differentiation of matrix elements satisfies both axioms.

Taking previous remarks in consideration, we suggest an alternative semantics for the derivative in the ZX-calculus. We use the fact that any parametrized ZX-diagram admits a linear map interpretation and the derivative of a parametrized linear map is well-defined. Therefore, in place of product rules we require the coherence between the derivatives in two categories related by an interpretation functor:

▶ **Definition 14** (Interpretation-coherent derivative)**.** *For two categories $\mathcal{A}, \mathcal{B}$ that are related by a standard interpretation $[\![-]\!] : \mathcal{A} \to \mathcal{B}$ a derivative ∂_A in $\mathcal{A}$ is an unary operator that commutes with the standard interpretation:*

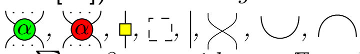
$$\forall D \in \mathcal{A} : \qquad [\![\partial_A D]\!] = \partial_B [\![D]\!] \tag{9}$$

where the category $\mathcal{B}$ is equipped with sum monoid and ∂_B is derivative in $\mathcal{B}$ satisfying the Definition 13.

In the context of ZX-diagrams, the Definition 14 requires the derivative of a parametrized diagram to map to the derivative of the corresponding matrix or, in other terms, to satisfy the property of *diagrammatic differentiation* [23].

4.1 Linear diagrams

Between parametrized diagrams, we distinguish the family of linear diagrams:

▶ **Definition 15** (Linear diagrams [14])**.** *A ZX-diagram is linear in $\beta_1, \ldots, \beta_k$ with constants in $L \subset \mathbb{R}$ if it is generated by*  *combined by tensor product and composition with α of the form $\sum_i n_i \beta_i + c$ with $n_i \in \mathbb{Z}$ and $c \in L$.*

It was shown in [14] that for $L = \{\frac{n\pi}{4}\}_{n \in \mathbb{Z}}$ the Clifford+T axiomatization (Figure 1) is complete for linear diagrams.

The family of linear diagrams may appear restricted compared to ZX-diagrams that allow angles from a more general class of functions. It is, however, sufficient for applications in variational quantum algorithms as they use circuits where parameters appear in a linear fashion [3]. More importantly, for this family we demonstrate simple formulas for the derivative. We believe that such formulas are not obtainable even for a slightly more general fragment $\mathrm{ZX}_{\mathcal{A}_n}$ where angles are in the group of affine functions $\mathcal{A}_n = \{(\beta) \to c^T\beta + c_0 | c \in \mathbb{R}^n, c_0 \in \mathbb{R}\}$. Intuitively, the difficulty comes from the absence of a simple representation for a general matrix over real numbers in terms of spiders. This restriction is removed in algebraic ZX-calculus [26] at the cost of an extended set of generators.

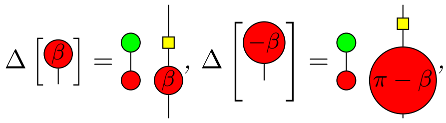
In order to keep the notations simple in what follows we restrict our attention to one-variable diagrams $\mathrm{ZX}(\beta)$. We denote the corresponding matrices by $\mathcal{M}(\beta)$. The derivative $\partial_M : \mathcal{M}(\beta) \to \mathcal{M}(\beta)$ is defined by entrywise application of the derivative $\partial_\beta : k\beta + c \mapsto k$. All results may be easily extended to the case of partial derivatives ∂_{β_i} for linear diagrams with an arbitrary number of variables.

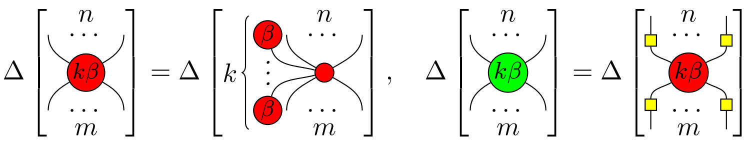
4.2 Diagrammatic differentiation with controlizers

The derivative in $\mathcal{M}(\beta)$ is defined through product rules that involve sums. In this section we use constructions from Section 3 to incorporate these rules in the diagrammatic framework.

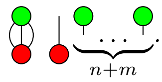
In what follows we denote by $C : \mathrm{ZX} \to \mathrm{ZX}$ any map that satisfies Definition 6 of controlizer.

▶ **Definition 16.** *We call C-derivative a map $\Delta : \mathrm{ZX}(\beta) \to \mathrm{ZX}(\beta)$ that associates to a diagram $D : n \to m$ another diagram $\Delta(D) : 1 \to n + m$ defined as follows:*

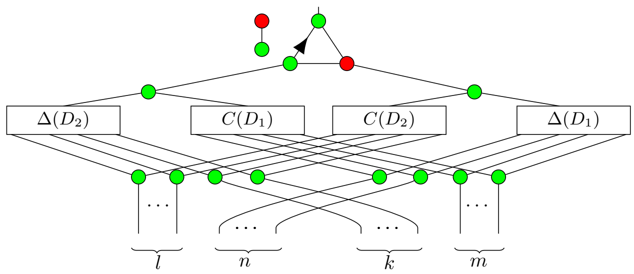
(i) ***Generators:*** *For parametrized spiders:* 



(10)

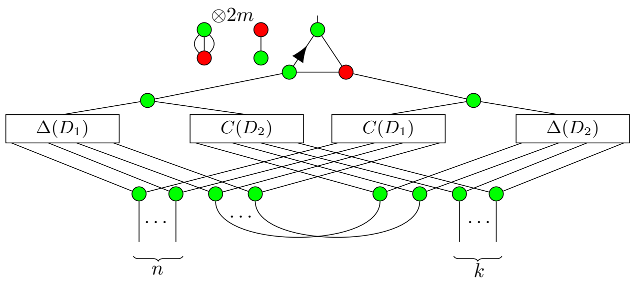
For all generators $g : n \to m$ that are independent on β $\Delta[g] =$ 

(ii) ***Tensor product:*** *for $D_1 : n \to m$ and $D_2 : l \to k$ the diagram $\Delta(D_2 \otimes D_1)$ is:*

$\Delta(D_2 \otimes D_1) =$ 

(11)

(iii) ***Composition:*** *for $D_1 : n \to m$ and $D_2 : m \to k$ the diagram $\Delta(D_2 \circ D_1)$ is:*

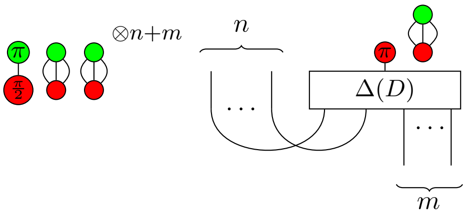
$\Delta(D_2 \circ D_1) =$ 

(12)

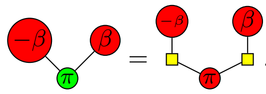
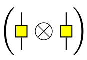
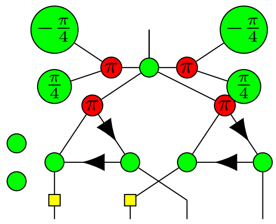
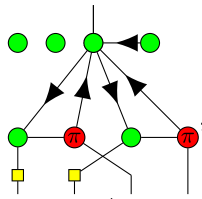
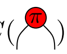
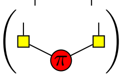
▶ Remark 17. It follows from Lemma 5 that for every diagram $D : n \to m$, $\Delta(D) : 1 \to n + m$ is a controlled state.

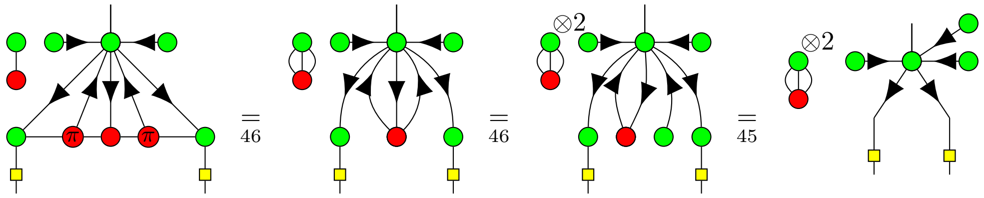
The Remark 9 on the dependency of the output on the decomposition order is also true for the map Δ.

▶ **Definition 18.** *Given the C-derivative Δ, let $\partial_C : \mathrm{ZX}(\beta) \to \mathrm{ZX}(\beta)$ be the unary operator such that for any diagram $D : n \to m$,*

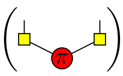
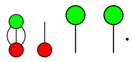
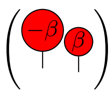
$\partial_C[D] =$  (13)

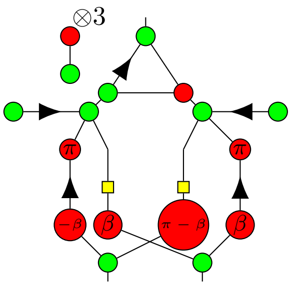
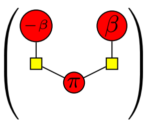
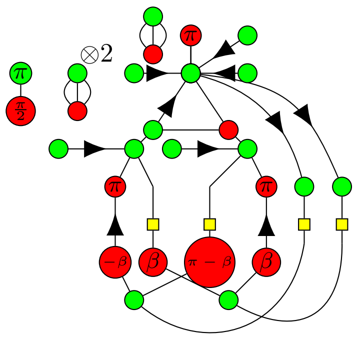
▶ **Theorem 19.** *The operator ∂_C satisfies the Definition 14 of diagrammatic differentiation.*

▶ **Example 20.** We apply Definition 18 to the simple diagram . Notice that C  $=$  $\underset{\substack{43\\(1)\\37}}{=}$ , moreover $C($$)$ was already found in Example 10. We obtain a diagram for C :



(14)

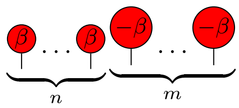
We know from Lemma 48 that Δ  $=$ . By definition, Δ  $=$

 and ∂_C  $=$ 

The last diagram may be further simplified. However, we show later (Example 30) that with our second approach a much simpler diagram for this expression may be obtained directly.

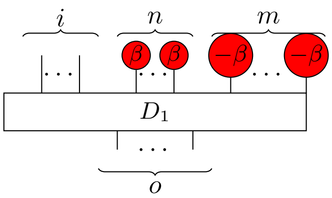
4.3 Formula for derivatives in $\mathrm{ZX}(\beta)$

Although perfectly correct, the differentiation procedure described above leads to very puzzling output even for small diagrams (see Example 20). In this section we provide a simpler approach to obtain the derivative of a diagram in $\mathrm{ZX}(\beta)$. We formalize it in definitions ∂_{ZX} and ∂_P of unary operators that satisfy the property of diagrammatic differentiation (Definition 14).

Let's denote by $X_\beta(n,m)$ diagrams  from $\mathrm{ZX}(\beta)$.

From the (S1) and (H) rules and the paradigm *Only topology matters* follows:

▷ Claim 21. Using the rules of ZX calculus, each diagram $D(\beta) : i \to o$ from $ZX(\beta)$ may be transformed into the form

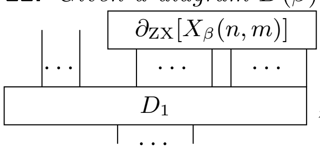
$D(\beta) =$  (15)

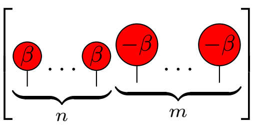
where n, m are some integer numbers and $D_1 : i + n + m \to o$ is constant with respect to β. We call diagrams in this form β-factored.

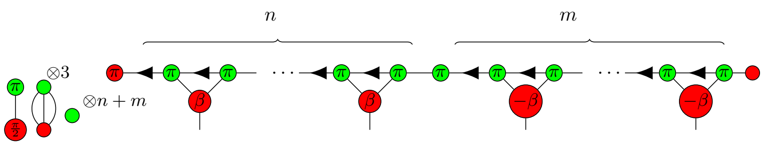
A rigorous demonstration of the claim 21 may be found in [14].

We define the derivative for diagrams in β-factored forms:

▶ **Definition 22.** *Given a diagram $D(\beta)$ in β-factored form, let*

$\partial_{\mathrm{ZX}}[D] =$  *, where*

$\partial_{\mathrm{ZX}}[X_\beta(n,m)] = \partial_{\mathrm{ZX}}$  $=$

$=$  (16)

▶ **Theorem 23.** *The operator $\partial_{\mathrm{ZX}}[-]$ from the Definition 22 satisfies the property of diagrammatic differentiation:*

For any diagram $D(\beta) \in \mathrm{ZX}(\beta)$ in β-factored form $[\![\partial_{\mathrm{ZX}} D(\beta)]\!] = \partial_M [\![D(\beta)]\!]$

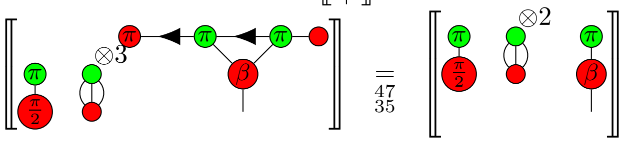
We remark that according to the Definition 14 the derivative $D' : n \to m$ of a diagram $D : n \to m$ that is constant on β is such that $[\![D']\!] = \partial_M [\![D]\!] = (0)_{n\times m}$. Therefore, Theorem 23 is a direct consequence of the following lemma:

▶ **Lemma 24.** *For any n, m:*

$$[\![\partial_{\mathrm{ZX}} X_\beta(n,m)]\!] = \partial_M [\![X_\beta(n,m)]\!] \tag{17}$$

Proof (Lemma 24). We prove the lemma by induction. The demonstration is done for the induction over n, the proof for m is directly obtainable in the same way.

Base. We show that $[\![\partial_{ZX} X_\beta(1,0)]\!] = \partial_M$  $= \partial_M \left(|+\rangle + e^{i\beta}|-\rangle\right) = ie^{i\beta}|-\rangle$. Indeed,

$[\![\partial_{ZX} X_\beta(1,0)]\!] =$  $= ie^{i\beta}|-\rangle$

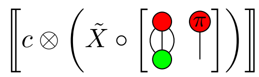
Step. By induction, we assume that the equation (17) holds for some n and m. We show that, under this assumption, $[\![\partial_{ZX} X_\beta(n+1,m)]\!] = \partial_M [\![X_\beta(n+1,m)]\!]$. The demonstration follows from the claims below:

▷ Claim 25.

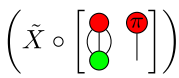
$$\partial_M [\![X_\beta(n+1,m)]\!] = [\![\partial_{ZX} [X_\beta(1,0)] \otimes X_\beta(n,m)]\!] + [\![X_\beta(1,0) \otimes \partial_{ZX} [X_\beta(n,m)]]\!] \tag{18}$$

where $(+)$ is the sum in $\mathcal{M}(\beta)$.

▷ Claim 26. We can find a controlled state $\tilde{X} : 1 \to n+1+m$ and a constant scalar $c \in \mathrm{ZX}_{\frac{\pi}{2}}$ such that

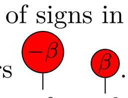
 $= [\![\partial_{ZX} [X_\beta(1,0)] \otimes X_\beta(n,m)]\!] + [\![X_\beta(1,0) \otimes \partial_{ZX} [X_\beta(n,m)]]\!]$ (19)

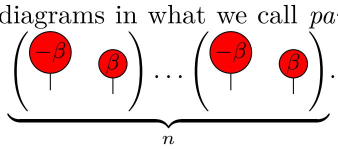
▷ Claim 27.

$\mathrm{ZX} \vdash \partial_{ZX} X_\beta(n+1,m) = c \otimes$  (20)

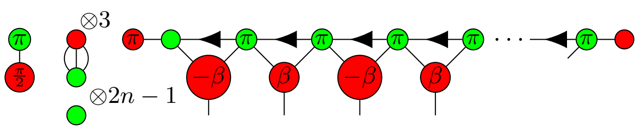
◀

4.4 Simplified formula for paired spiders

Variational quantum algorithms use gradients in the search for optimal parameter values. The objective minimized by these algorithms can be expressed as $\langle\psi(\beta)|H|\psi(\beta)\rangle$ where the diagram for $\langle\psi(\beta)| = (|\psi(\beta)\rangle)^\dagger$ is obtained out of the diagram for $|\psi(\beta)\rangle$ by flipping up side down followed by the change of signs in spiders. Therefore, parameters in the diagram for $\langle\psi(\beta)|H|\psi(\beta)\rangle$ appear in pairs .

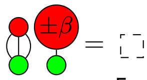
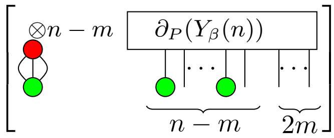
We suggest a more compact formula for diagrams in what we call *pair-factored form*: $D_2 \circ (D_1 \otimes Y(n))$. In this expression $Y_\beta(n) =$ .

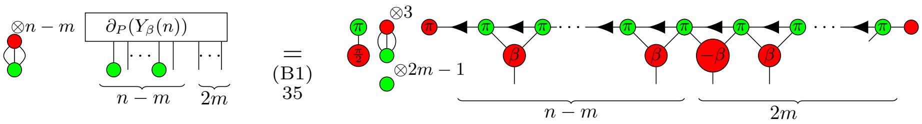
▶ **Lemma 28.** *The diagram:*

$\partial_P(Y_\beta(n)) =$  (21)

satisfies $[\![\partial_P(Y_\beta(n))]\!] = \partial_M [\![Y_\beta(n)]\!]$.

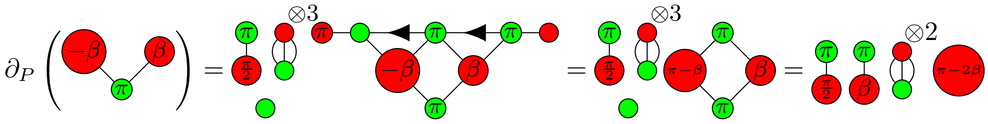
We prove Lemma 28 by applying the same approach as in the proof of Lemma 24. We can then replace by (21) the expression (16) in Definition 22 and obtain the derivative for diagrams in pair-factored form.

▶ **Observation 29.** *It is possible to extend Lemma 28 to find the derivative for* $X_\beta(n,m)$ *when* $n \neq m$*. Indeed, using the fact that*  *we can balance the number of* β *and* $-\beta$*. For instance, if* $n > m$*:* $\partial_P\left(X_\beta(n,m)\right) = \sigma \circ$  *where* σ *is some wire permutation and*



(22)

▶ **Example 30.** We apply Lemma 28 to the same diagram as in Example 20:



(23)

5 Diagrammatic representation of Ising Hamiltonians

Parametrized quantum circuits are the main component of quantum-classical variational algorithms such as QAOA [7] and VQE [20]. These algorithms are designed to (approximately) solve problems of optimization over binary variables:

$$\min_{x\in\{0,1\}^n} f(x) \tag{24}$$

In order to be treated by a quantum computer an instance $f : \{0,1\}^n \to \mathbb{R}$ of the optimization problem (24) is encoded in a Hamiltonian - an operator H_f acting on qubit states. The Hamiltonian is diagonal in computational basis, $H_f : |x\rangle \to f(x)|x\rangle$. The ground state of H_f corresponds to the optimum of the problem.

For every input Hamiltonian H_f a quantum-classical optimization algorithm starts by designing an anzatz $Q_f(\beta) : n \to n$ [3]. An anzatz is a parametrized quantum circuit with blocks that (possibly) depend on H_f. Classical optimization is used to determine the values $\hat{\beta}$ that minimize the expectation of the Hamiltonian $\langle\psi(\hat{\beta})|H_f|\psi(\hat{\beta})\rangle$ [7].

Many important optimization problems such as *Maximum Cut* and *Maximum Independent Set* in a graph may be encoded in so called Ising Hamiltonians [18]:

▶ **Definition 31.** *An Ising Hamiltonian* $H : n \to n$ *with integer coefficients is an operator:*

$$H = \sum_{1\le i\le n} h_i Z_i + \sum_{1\le i<j\le n} h_{ij} Z_i Z_j, \quad h_i, h_{ij} \in \mathbb{Z} \tag{25}$$

where Z_i *denotes Pauli-Z gate acting on the qubit* i*.*

We observe that there is no direct way to transform the definition of the Hamiltonian (31) to a ZX-diagram. Indeed, Hamiltonian is a non-unitary matrix equal to a *sum* of Pauli gates that is inherently difficult to represent as a diagram. So far, all attempts in this direction used formal sums of diagrams [23, 28]. As a consequence, the application of ZX-calculus to variational algorithms was limited. We show how our formula (16) allows to find a diagram for an Ising Hamiltonian H.

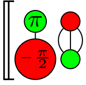
Firstly, we remark that for an Ising Hamiltonians H the diagram $D_U(\beta)$ of the linear map $U(\beta) = e^{i\beta H}$ is easy to find [24]. For Hamiltonians with integer coefficients the matrix $U(\beta) = e^{i\beta H}$ belongs to $\mathcal{M}(\beta)$. It satisfies the definition of strongly continuous one-parameter unitary group:

▶ **Definition 32** (Unitary group [23]). *A one-parameter unitary group is a unitary matrix $U : n \to n$ in $\mathcal{M}(\beta)$ with $U(0) = id_n$ and $U(\beta)U(\beta') = U(\beta + \beta')$ for all $\beta, \beta' \in \mathbb{R}$. It is strongly continuous when $\lim_{\beta \to \beta_0} U(\beta) = U(\beta_0)$ for all $\beta_0 \in \mathbb{R}$.*

▶ **Theorem 33** (Stone ([22])). *There is a one-to-one correspondence between strongly continuous one-parameter unitary groups $U : n \to n$ in $\mathcal{M}(\beta)$ and self-adjoint matrices $H : n \to n$ in $\mathcal{M}$. The bijection is given explicitly by $U(\beta) = e^{i\beta H}$ and $H = -i(\partial_M U)(0)$.*

We use the bijection from the Stone's theorem to find the diagram $h \in ZX_{\mathbb{R}}$ such that $[\![h]\!] = H$. Using the property $U(0) = \mathrm{id}_n$ we obtain:

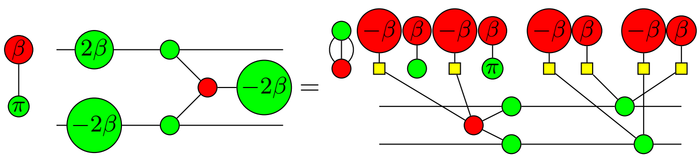
$$H = -i[\partial_M U(\beta)](0) = -i \otimes [\![[\partial_{\mathrm{ZX}} D_U](\beta)]\!](0) = -i \otimes [\![[\partial_{\mathrm{ZX}} D_U](0)]\!]$$

$= \Bigg[\!\!\Bigg[$  $[\partial_{\mathrm{ZX}} D_U](0) \Bigg]\!\!\Bigg] = [\![h]\!]$ (26)

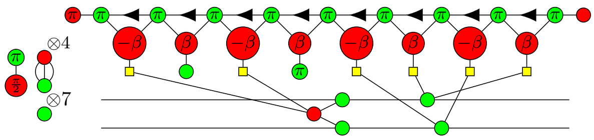
where the third equality is due to the fact that the evaluation commutes with the standard interpretation.

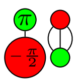
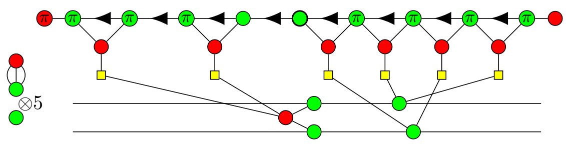
We give an example of diagram for an Ising Hamiltonian obtained via our approach.

▶ **Example 34.** Let $H : 2 \to 2$, $H = Z_1 - Z_2 + Z_1 Z_2$. The diagram $D_U(\beta)$ for $U(\beta) = e^{i\beta H}$ is:

$D_U(\beta) =$  (27)

Using the formula (21) we find the derivative of $D_{U(\beta)}$:

$\partial_{\mathrm{ZX}} D_{U(\beta)} =$  (28)

$h =$  $[\partial_{\mathrm{ZX}} D_{U(\beta)}]_{\beta \to 0} =$  (29)

6 Discussions

In this work, we have introduced for the first time an inductive definition for addition of ZX-diagrams, that we have then used to introduce an inductive definition of the differentiation of ZX-diagrams. Addition and differentiation are essential tools for the development and the study of quantum algorithms, but, as a matter of fact, both of them are leading to large diagrams, even when the initial diagrams are fairly simple. From a process theory point of view, contrary to sequential and parallel compositions, the addition is not physical operation, hence it is not surprising that it is not a native or simple operation over ZX-diagrams. The good news is that we can rely on the powerful equation theory of the ZX-calculus to simplify, when it is possible, the diagrams representing the sum or the differentiation of diagrams.

In Section 4.3, we have shown that instead of simplifying the resulting diagrams *a posteriori*, one can *a priori* put the initial diagrams in an appropriate form. While this approach is not inductive anymore, it seems to ease the differentiation of diagrams in practice. Notice that this last approach, in particular Definition 22, leads to a very similar differentiation of diagrams to the one independently introduced in [27]. In their work, the authors directly introduce the differentiation of ZX-diagrams in some particular form, in contrast to the inductive definition we propose, but another important difference is actually the diagrammatic language and its expressivity. While our work is based on the "vanilla" ZX-calculus, the authors of [27] rely on the algebraic ZX-calculus, i.e. a ZX-calculus augmented with boxes allowing, roughly speaking, the direct representation of a complex numbers, whereas only angles can be used as parameters in the vanilla ZX-calculus. As a consequence when an algebraic ZX-diagram is parameterised by an arbitrary derivable function $f(x)$, the differentiated algebraic ZX-diagram is parametrised by $f'(x)$. Such an approach is not possible in the more constrained vanilla ZX-calculus thus we restrict our attention to a family of functions (essentially the linear ones) which derivative can be expressed using the structure of the vanilla ZX-calculus.

In most practical examples the vanilla ZX-calculus is sufficient to represent parametrised computation. As an application we have shown that our result allows the construction of diagrams for Ising Hamiltonians and for derivatives of parametrized circuits. Therefore, it becomes possible to study variational algorithms entirely within the ZX-calculus. In particular, we can use rewrite rules to simplify such expressions as $\langle\psi(\hat{\beta})|H_f|\psi(\hat{\beta})\rangle$ and $\frac{\partial\langle\psi(\hat{\beta})|H_f|\psi(\hat{\beta})\rangle}{\partial\beta}$. We believe that it will lead to a better understanding of the potential of variational algorithms and of their applications to real-world problems.

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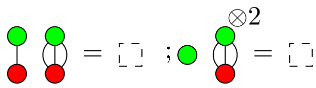
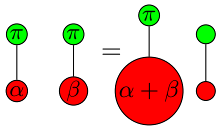
A ZX lemmas

A.1 Already proven lemmas [15]

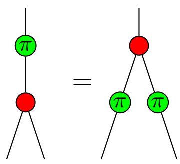
▶ **Lemma 35.**



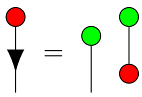
▶ **Lemma 36.**



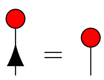
▶ **Lemma 37.**



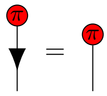
▶ **Lemma 38.**



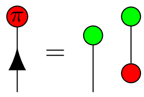
▶ **Lemma 39.**



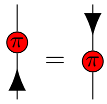
▶ **Lemma 40.**



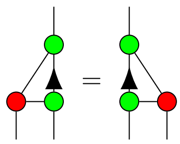
▶ **Lemma 41.**



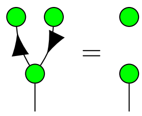
▶ **Lemma 42.**



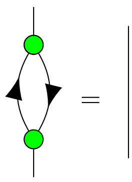
▶ **Lemma 43.**



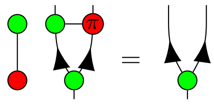
▶ **Lemma 44.**



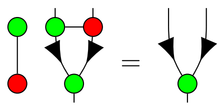
▶ **Lemma 45.**



▶ **Lemma 46.**

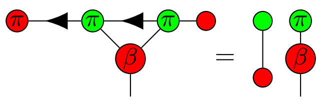


and

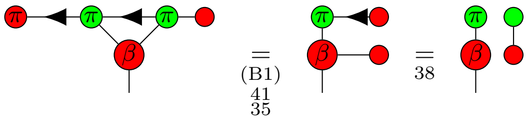


A.2 New lemmas

▶ **Lemma 47.**

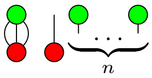
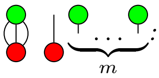


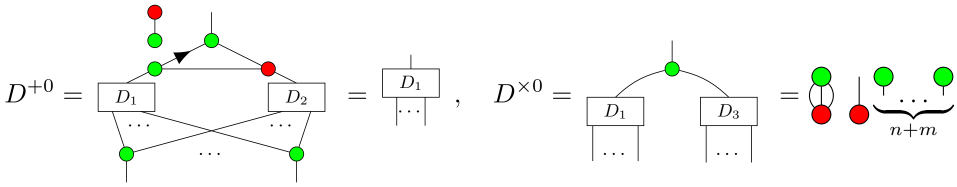
Proof.

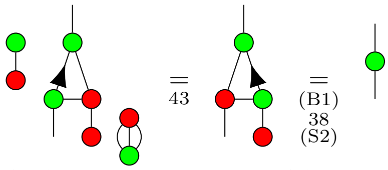


(30)

◀

▶ **Lemma 48.** *For all controlled states $D : 1 \to n$ and states D_2, D_3 that are $D_2 =$*  *and $D_3 =$* *:*



Proof. The equality for D^{+0} holds as 

The equality for $D^{\times 0}$ follows from (B1) and the definition (3) of controlled states. ◀