

Differentiating and Integrating ZX Diagrams with Applications to Quantum Machine Learning

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ZX-calculus has proved to be a useful tool for quantum technology with a wide range of successful applications. Most of these applications are of an algebraic nature. However, other tasks that involve differentiation and integration remain unreachable with current ZX techniques. Here we elevate ZX to an analytical perspective by realising differentiation and integration entirely within the framework of ZX-calculus. We explicitly illustrate the new analytic framework of ZX-calculus by applying it in context of quantum machine learning for the analysis of barren plateaus.

1 Introduction

ZX-calculus is a powerful graphical rewrite system proposed by Coecke and Duncan [11] for linear maps, particularly for quantum circuits. A node with n edges in a ZX diagram, like in tensor network notation, represents an order n tensor. Moreover, it is possible to directly evaluate the tensor by performing local rewrites (i.e., substitution of a part of a ZX diagram). Using these local rewrites, ZX-calculus has been successfully applied to circuit compilation [4, 5, 18, 43], measurement-based quantum computing [27, 19], fusion-based quantum computing [8], quantum error correction [26, 6], quantum natural language processing [14, 34, 25], and quantum foundations [2, 13, 12, 20]. ZX-calculus can even be used as a concrete realisation of quantum theory [15]. These applications of ZX-calculus are algebraic in nature, and take advantage of *rewriting as a form of computation*: in fact ZX-calculus is a sound, universal [10] and complete [23] proof system that serves as an alternative to traditional linear algebra, which also makes it a different formalism from tensor networks. However, without the analytical tools of differentiation and integration, ZX-calculus fell short of tackling variational problems such as quantum machine learning or realising a comprehensive version of quantum mechanics including quantum dynamics.

In this paper we give for the first time rules for differentiating arbitrary ZX diagrams and integrating a wide class of ZX diagrams (including quantum circuits), within the framework of a slightly extended version of ZX-calculus called algebraic ZX-calculus [47] which makes it very convenient to deal with sums of ZX diagrams, thus paving the way for an analytical version of ZX-calculus. We apply these new techniques to develop a framework for a purely ZX-based analysis of the barren plateau phenomenon from quantum machine learning.

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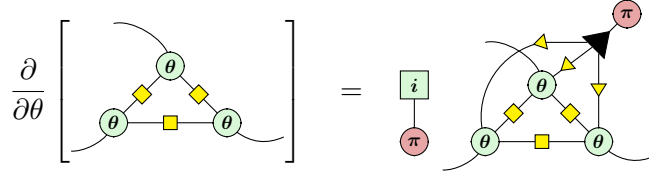


Figure 1: Example of diagrammatic differentiation.

Related Work

There have been previous attempts at providing rules for differentiating and integrating ZX diagrams [51, 45, 52]. In particular, Zhao and Gao [52] pioneered the use of ZX-calculus to aid in the analysis of the barren plateau phenomenon. Similar techniques were also used in [36] to study quantum tensor network ansätze. However, by explicitly using Hilbert space operations such as addition, all these previous attempts fall outside the realm of vanilla ZX-calculus as there are few techniques to further manipulate sums of diagrams. Ultimately, all previous works studying barren plateaus in the ZX-calculus had to resort to a combination of ZX diagrams and general tensor networks in order to handle this summation problem. The analytical ZX techniques developed in this paper on the other hand offer a unified framework to reason about differentiation and integration purely in terms of rewriting, without having to fall back to arbitrary tensor networks.

Previous attempts to formalise sums of ZX diagrams include work by Stollenwerk and Hadfield [44] who provide notation for representing sums of ZX diagrams as a single diagram by extending the ZX calculus with a pair of sum boxes which were later formalised by Villoria, Baisold, and Laarman [46]. However, this approach does not offer much additional diagrammatic reasoning power since it is merely syntactic sugar for writing linear combinations of diagrams. Jeandel, Perdrix, and Veshchezerova [24] independently derived an alternate method to represent sums and derivatives with the ZX-calculus by showing how the sum of two controlled ZX diagrams can be represented as a single controlled ZX diagram. However, their approach requires an inductive translation of diagrams to controlled diagrams such that the result will not resemble the original diagram. Our method on the other hand preserves diagram structure and can be calculated almost instantly. We refer to Appendix D for a more thorough comparison of the two approaches.

Finally, our approach also offers a numerical advantage: The tensor networks considered in [52, 36] have bond dimension 3 whereas all our diagrams only have dimension 2, yielding a speed-up when contracting the diagram in software. This was exploited in [31] to numerically detect the presence of barren plateaus by contracting diagrams representing the gradient variance of ansätze and observing the decay. Crucially, that work builds on our diagrammatic barren plateau framework developed in this paper, making use of the more efficient 2-dimensional representation compared to [52, 36]. Furthermore, the techniques developed in our work have QML applications beyond barren plateaus. For example, our results have been used in [30] to analyse and derive novel parameter shift rules for gradient computation using ZX.

Summary of results

1. Differentiation of arbitrary (algebraic) ZX diagrams, with a unified diagrammatic chain and product rule. (Theorem 14 and Theorem 16)
2. Definite integration of circuit-like ZX diagrams, with up to 3 occurrences of a parameter. (Proposition 32, Theorem 33, and Theorem 34)

3. Diagrammatic formula for the expectation and variance of a quantum circuit's gradient $\frac{\partial \langle H \rangle}{\partial \theta_i}$. (Lemma 35 and Theorem 38)
4. Demonstration of barren plateau analysis for an example ansatz. (Section 5.2)

From a general ZX-calculus perspective, this is the first paper to combine sums of ZX diagrams into a single ZX diagram in a methodical way. In particular, we highlight the importance of the W spider in ZX-calculus, which corresponds to the derivation structure of the product rule. These results required the combined power of the Z, X and W spiders, all 3 of which can be naturally represented within algebraic ZX-calculus.

Note: For presentation purposes, the proofs of some theorems and lemmas are moved to the appendix.

2 Algebraic ZX-calculus

The generators of the original ZX-calculus [11] are chosen with the aim to conveniently represent quantum computational models using complementary observables. On the other hand, the ZW-calculus [22] is designed based on the GHZ and W states, two maximally entangled quantum states [16]. It is known that the Z and W spiders from ZW-calculus act as the multiplication and addition monoid respectively, making it possible to perform arithmetic [17, 22].

We will see that the W state is crucial for dealing with sums of diagrams, and it is in fact closely related to the product rule used in differentiation. Conveniently, algebraic ZX-calculus [47] compactly decomposes the W spider and other gadgets such as the logical AND gate [38], into Z spiders, X spiders and triangle gates, thus giving us the benefits of ZX and ZW calculus within a single unified framework.

The yellow triangle of algebraic ZX-calculus is powerful as it sends the computational basis to a non-orthogonal basis, which makes diagrammatic representation and calculation of other logical gates much simpler. Conversely, the representation of the yellow triangle using other graphical calculi is more complicated. Intuitively, this is because the triangle gate is a low-level primitive in comparison to the Z, X, W and H spiders [3]. This algebraic extension of ZX is a universal and complete language for not just complex numbers, but also commutative rings and semirings [49].

In this section, we give an introduction to the algebraic ZX-calculus, including its generators and rewriting rules. In this paper ZX diagrams are either read from left to right or top to bottom.

2.1 Generators

The diagrams in algebraic ZX-calculus are defined by freely combining the following generating objects:

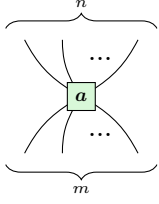
$R_{Z,a}^{(n,m)} : n \rightarrow m$		$\mathbb{I} : 1 \rightarrow 1$	
$H : 1 \rightarrow 1$		$\sigma : 2 \rightarrow 2$	
$C_a : 0 \rightarrow 2$		$C_u : 2 \rightarrow 0$	
$T : 1 \rightarrow 1$		$T^{-1} : 1 \rightarrow 1$	

Table 1: Generators of algebraic ZX-calculus, where $m, n \in \mathbb{N}$, $a \in \mathbb{C}$.

2.2 Additional notation

For simplicity, we introduce additional notation based on the given generators:

1. The green spider from the original ZX-calculus can be defined using the green box spider in algebraic ZX-calculus.

$$\begin{array}{ccc} \text{Green spider with } \alpha & := & \text{Green box spider with } e^{i\alpha} \\ \text{Green spider with } 1 & := & \text{Green box spider with } 1 \end{array}$$

2. The whitespace around a diagram can be interpreted as an explicit horizontal composition with the empty diagram.

$$\begin{array}{ccc} \text{Empty box} & := & \text{Empty box} \end{array}$$

3. The transposes of the triangle and the inverse triangle can be drawn as an inverted triangle.

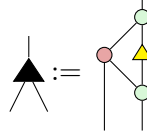
$$\begin{array}{ccc} \text{Yellow triangle up} & := & \text{Yellow triangle down} \\ \text{Yellow triangle down} & := & \text{Yellow triangle up}^{-1} \end{array}$$

4. The pink spider is the algebraic equivalent of the red spider from the original ZX-calculus. It is only defined for $\tau \in \{0, \pi\}$, and is rescaled to have integer components in its matrix representation.

$$\begin{array}{ccc} \text{Pink spider with } \tau & := & \text{Green box spider with } \left(2^{\frac{m+n-2}{2}} - 1 \right) \tau \text{ and } (X) \\ \text{Pink spider with } 0 & := & \text{Pink spider with } 0 \end{array}$$

Note that the green box represents the scalar $\left(2^{\frac{m+n-2}{2}} - 1 \right) \tau = 2^{\frac{m+n-2}{2}}$.

5. The W spider from ZW-calculus can be expressed as follows.



2.3 Interpretation

Although the generators in ZX-calculus are formal mathematical objects in their own right, in the context of this paper we interpret the generators as linear maps, so each ZX diagram is equivalent to a vector or matrix. For $a \in \mathbb{C}$, we have

$$\underbrace{\text{Diagram with } a \text{ in a box}}_m^n = |0\rangle^{\otimes m} \langle 0|^{\otimes n} + a |1\rangle^{\otimes m} \langle 1|^{\otimes n}, \quad (Z)$$

$$\text{Yellow square} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \text{Yellow triangle} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \quad \text{Yellow triangle}^{-1} = \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}$$

$$| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \text{Cup} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad \text{Cap} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Furthermore, parallel and sequential composition of diagrams correspond to matrix multiplication and tensor product of the underlying linear maps, respectively. Using the interpretation of these generators, we can compute the matrices for other frequently occurring diagrams by composition:

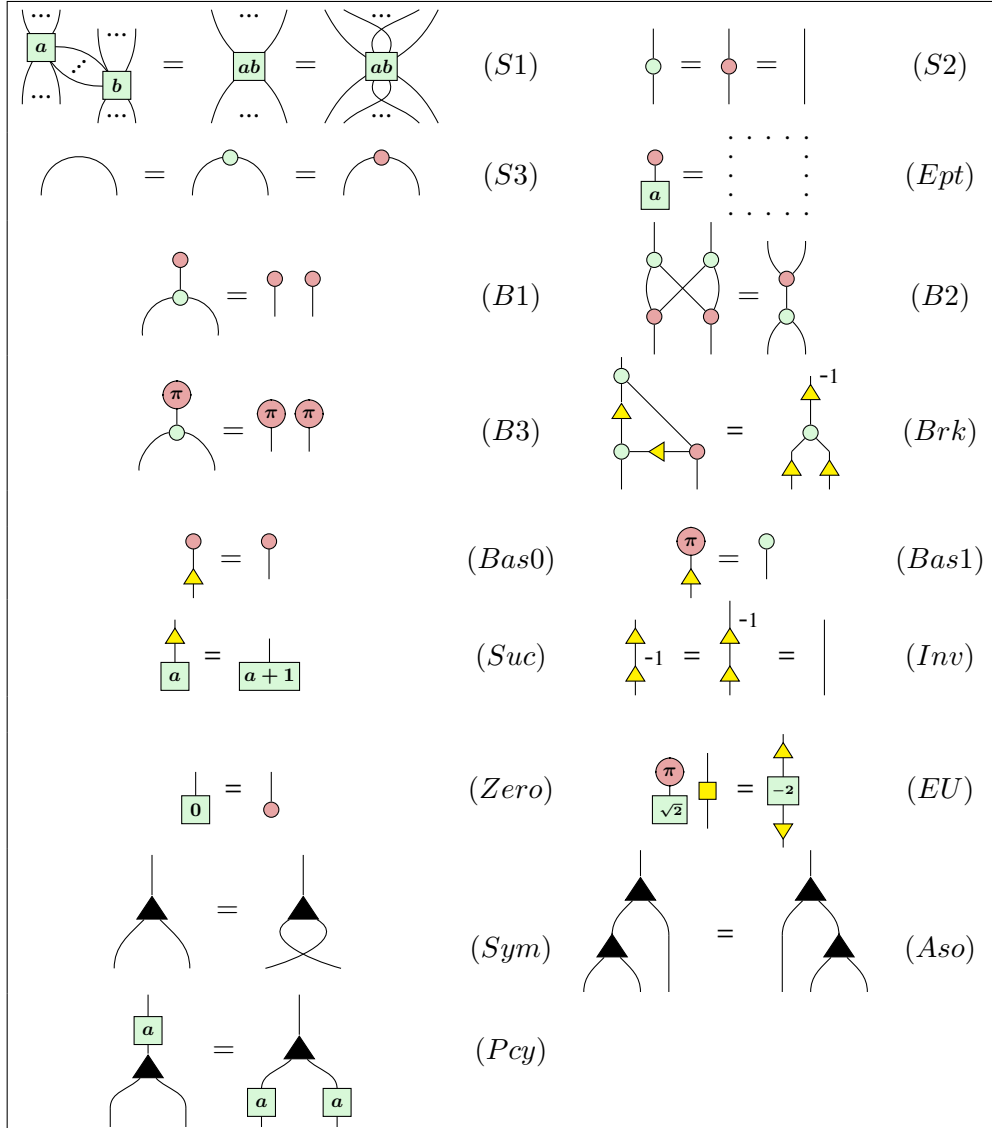
$$\underbrace{\text{Diagram with } k\pi \text{ in a box}}_m^n = \sum_{\substack{0 \leq i_1, \dots, i_m, j_1, \dots, j_n \leq 1 \\ i_1 + \dots + i_m + k \equiv j_1 + \dots + j_n \pmod{2}}} |i_1, \dots, i_m\rangle \langle j_1, \dots, j_n|, \quad k \in \{0, 1\},$$

$$\text{Red circle} = |0\rangle, \quad \text{Red circle} = \langle 0|, \quad \text{Red circle with } \pi = |1\rangle, \quad \text{Red circle with } \pi = \langle 1|, \quad \text{Red circle with } \pi = 0, \quad \text{Red circle with } \pi \text{ and } a \text{ in a box} = \boxed{a-1} = a.$$

$$\text{Red circle with } \pi = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \text{Green circle with } \alpha \text{ and yellow squares} = e^{i\frac{\alpha}{2}} \begin{pmatrix} \cos \frac{\alpha}{2} & -i \sin \frac{\alpha}{2} \\ -i \sin \frac{\alpha}{2} & \cos \frac{\alpha}{2} \end{pmatrix}, \quad \text{Box with } a = 1.$$

2.4 Rules

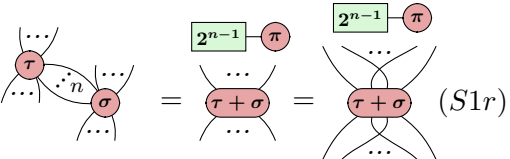
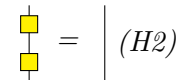
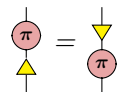
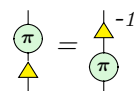
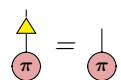
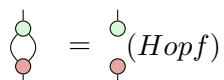
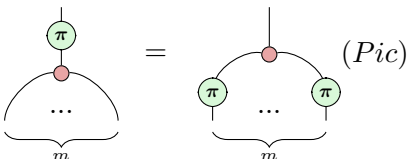
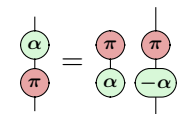
Now we give the rewriting rules of algebraic ZX-calculus.



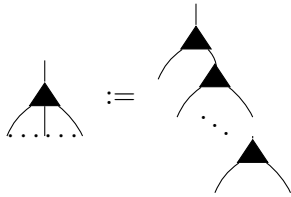
Where $a, b \in \mathbb{C}$. The vertically flipped versions of the rules are assumed to hold as well.

2.5 Useful lemmas

The following lemmas which will be used in the sequel can be derived from the rules.

Lemma 1. [48] For $\tau, \sigma \in \{0, \pi\}$, pink spiders fuse. 	Lemma 2. [48] Hadamard is involutive. 
Lemma 3. [48] Pink π transposes the triangle. 	Lemma 4. [48] Green π inverts the triangle. 
Lemma 5. [48] triangle stabilises $\langle 1$. 	Lemma 6. [48] Hopf rule. 
Lemma 7. [48] π copy rule. For $m \geq 0$: 	Lemma 8. [48] π commutation rule. 

Remark 9. Due to the associative rule (Aso), we can define the W spider



and give its interpretation as follows [21]:

$$\underbrace{\text{triangle}}_m = \underbrace{|0 \cdots 0\rangle}_m \langle 0| + \sum_{k=1}^m \underbrace{|0 \cdots 0 1 0 \cdots 0\rangle}_{k-1} \langle 1|.$$

As a consequence, we have

$$\begin{aligned}
 \text{Diagram 1} &= \text{Diagram 2} \\
 \text{Diagram 3} &= \text{Diagram 4} + \text{Diagram 5} + \dots + \text{Diagram 6}
 \end{aligned}
 \tag{1}$$

For $n = 2$, the state $|01\rangle + |10\rangle$ can be represented as the quantum state corresponding to the Pauli X gate according to the map-state duality:

Lemma 10.

$$\text{Diagram 7} = \text{Diagram 8}$$

3 Differentiating ZX diagrams

In this section, we show how to differentiate any algebraic ZX diagram within algebraic ZX-calculus, and how to represent the derivative of original ZX diagrams [11] and quantum circuits in algebraic ZX as a special case. We refer to [45] for a formal definition of the categorical semantics of diagrammatic differentiation. We start by differentiating the simplest parameterised generator in original ZX-calculus: the one-legged green spider.

Lemma 11. Suppose $f(\theta)$ is a differentiable real function of θ . Then

$$\frac{\partial}{\partial \theta} \left[\text{Diagram 9} \right] = \text{Diagram 10}$$

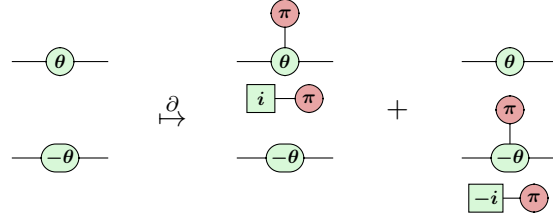
Note: For presentation purposes, the proofs of some theorems and lemmas are moved to the appendix.

Using the derivative of the one-legged spider, we can differentiate any ZX diagram with only one occurrence of the parameter being differentiated against. Here is an example.

$$\text{Diagram 11} = \text{Diagram 12} \xrightarrow{\partial} \text{Diagram 13} \stackrel{B3}{=} \text{Diagram 14}$$

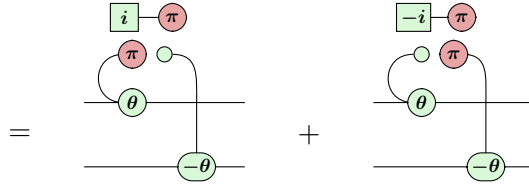
$$|00\rangle \langle 0| + e^{i2\theta} |11\rangle \langle 1| \xrightarrow{\partial} 2i * e^{i2\theta} |11\rangle \langle 1|$$

When there are multiple occurrences of the same parameter, the derivative can be expressed as a sum of ZX diagrams using the product rule. For example, the density matrix of $R_z(\theta)$ can be differentiated as follows.

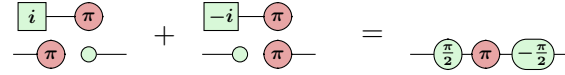


Since there are no rules on how to further manipulate sums of ZX diagrams, any reasoning from this point on would need to explicitly rely on the matrix interpretation of the diagrams instead of rewriting. In order to proceed with diagrammatic reasoning, we need to express the derivative as a single diagram.

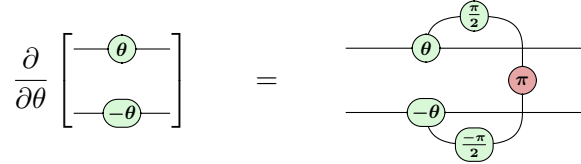
By observing that the product rule leaves the unparameterised parts of the diagram untouched and can be “factored out”, we only need to resynthesise the derivative of the parameterised part.



After this factorisation, the diagrammatic terms in the sum (top of the diagram) can be further manipulated until we can eliminate the sum using a simple rule such as $|0\rangle + |1\rangle = \sqrt{2}|+\rangle$. (See appendix for a demonstration of this technique)



Therefore



This equation, first derived by Zhao et al. [52], is essentially the parameter shift rule by Schuld et al. [40] expressed as a single ZX diagram (also see Corollary 18).

The key result of the paper allows us to express the derivative of an arbitrary ZX diagram in terms of a single diagram. It is based on the observation that the product rule and the unnormalised $|W_n\rangle$ state resemble each other: in the product rule, each term has one differentiated function, and in the W state each term has one bit set to 1 in the basis state.

$$\partial(fgh) = (\partial f)gh + f(\partial g)h + fg(\partial h)$$

$$|W_3\rangle = |100\rangle + |010\rangle + |001\rangle$$

We will show in Theorem 16 that the product rule can indeed be represented using a W state supplemented with some local change of bases. The following lemma demonstrates that the difference between f and ∂f can be expressed as a change of basis from the computational basis $|0\rangle, |1\rangle$.

Lemma 12. *For any complex number a , we have*

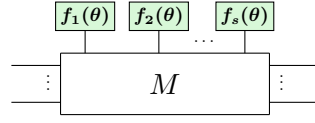


To differentiate algebraic ZX diagrams, we first differentiate its parameterised generator, the one-legged green box:

Lemma 13. *Suppose $f : \mathbb{R} \rightarrow \mathbb{C}$ is a differentiable function. Then*

$$\frac{\partial}{\partial \theta} \left[\begin{array}{c} \boxed{f(\theta)} \\ | \\ \text{---} \end{array} \right] = \begin{array}{c} \boxed{f'(\theta)} \quad \pi \\ | \quad | \\ \pi \quad \text{---} \end{array}$$

All parameterised differentiable algebraic ZX diagrams can be rewritten into the following form, where M is an unparameterised ZX diagram with respect to θ , and $\{f_i(\theta)\}_i$ are differentiable real functions of θ . Parameterised green spiders can be written as a green box with an exponentiated phase, and parameterised red spiders can be converted to parameterised green spiders via Hadamard conjugation. We emphasise that M can contain other parameterised spiders, just not with respect to θ .

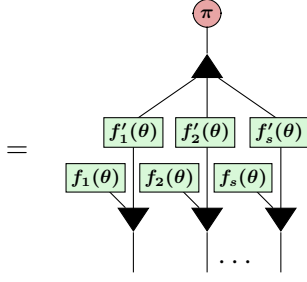


Theorem 14. *Assume $f_j : \mathbb{R} \rightarrow \mathbb{C}$ are differentiable functions. Then*

$$\frac{\partial}{\partial \theta} \left[\begin{array}{c} \boxed{f_1(\theta)} \quad \boxed{f_2(\theta)} \quad \boxed{f_s(\theta)} \\ | \quad | \quad | \\ \vdots \quad \vdots \quad \vdots \\ \boxed{M} \\ | \quad | \quad | \\ \vdots \quad \vdots \quad \vdots \end{array} \right] = \begin{array}{c} \pi \\ \swarrow \quad \downarrow \quad \searrow \\ \boxed{f'_1(\theta)} \quad \boxed{f'_2(\theta)} \quad \boxed{f'_s(\theta)} \\ | \quad | \quad | \\ \boxed{f_1(\theta)} \quad \boxed{f_2(\theta)} \quad \boxed{f_s(\theta)} \\ | \quad | \quad | \\ \vdots \quad \vdots \quad \vdots \\ \boxed{M} \\ | \quad | \quad | \\ \vdots \quad \vdots \quad \vdots \end{array}$$

Proof. By linearity, differentiating the overall diagram amounts to differentiating the parameterised part of the diagram:

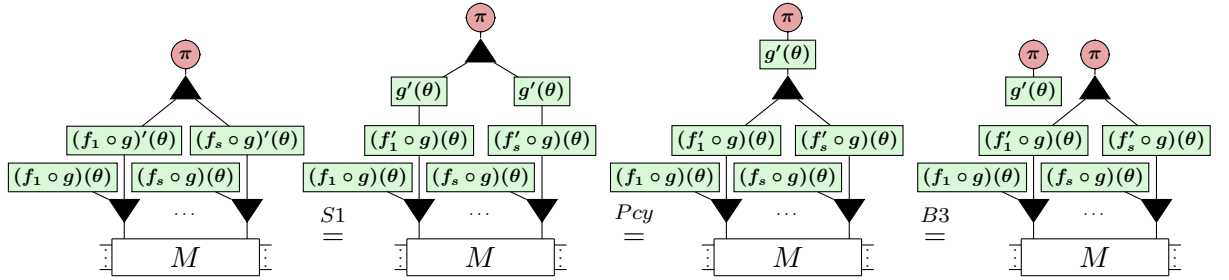
$$\begin{aligned} & \frac{\partial}{\partial \theta} \left[\begin{array}{c} \boxed{f_1(\theta)} \quad \boxed{f_2(\theta)} \quad \boxed{f_s(\theta)} \\ | \quad | \quad | \\ \vdots \quad \vdots \quad \vdots \end{array} \right] \\ &= \begin{array}{c} \boxed{f'_1(\theta)} \quad \pi \\ | \quad | \\ \pi \quad \text{---} \end{array} \begin{array}{c} \boxed{f_2(\theta)} \quad \boxed{f_s(\theta)} \\ | \quad | \\ \vdots \quad \vdots \end{array} + \begin{array}{c} \boxed{f'_2(\theta)} \quad \pi \\ | \quad | \\ \pi \quad \text{---} \end{array} \begin{array}{c} \boxed{f_1(\theta)} \quad \boxed{f_s(\theta)} \\ | \quad | \\ \vdots \quad \vdots \end{array} + \dots + \begin{array}{c} \boxed{f'_s(\theta)} \quad \pi \\ | \quad | \\ \pi \quad \text{---} \end{array} \begin{array}{c} \boxed{f_1(\theta)} \quad \boxed{f_2(\theta)} \\ | \quad | \\ \vdots \quad \vdots \end{array} \\ &= \begin{array}{c} \pi \quad \pi \quad \pi \\ | \quad | \quad | \\ \boxed{f_1(\theta)} \quad \boxed{f_2(\theta)} \quad \boxed{f_s(\theta)} \\ | \quad | \quad | \\ \boxed{f'_1(\theta)} \quad \boxed{f'_2(\theta)} \quad \boxed{f'_s(\theta)} \\ | \quad | \quad | \\ \pi \quad \text{---} \quad \text{---} \end{array} + \begin{array}{c} \pi \quad \pi \quad \pi \\ | \quad | \quad | \\ \boxed{f_1(\theta)} \quad \boxed{f_2(\theta)} \quad \boxed{f_s(\theta)} \\ | \quad | \quad | \\ \boxed{f'_2(\theta)} \quad \boxed{f'_1(\theta)} \quad \boxed{f'_s(\theta)} \\ | \quad | \quad | \\ \pi \quad \text{---} \quad \text{---} \end{array} + \dots + \begin{array}{c} \pi \quad \pi \quad \pi \\ | \quad | \quad | \\ \boxed{f_1(\theta)} \quad \boxed{f_2(\theta)} \quad \boxed{f_s(\theta)} \\ | \quad | \quad | \\ \boxed{f'_1(\theta)} \quad \boxed{f'_2(\theta)} \quad \boxed{f'_s(\theta)} \\ | \quad | \quad | \\ \pi \quad \text{---} \quad \text{---} \end{array} \\ &= \begin{array}{c} \pi \quad \pi \quad \pi \\ | \quad | \quad | \\ \boxed{f'_1(\theta)} \quad \boxed{f'_2(\theta)} \quad \boxed{f'_s(\theta)} \\ | \quad | \quad | \\ \boxed{f_1(\theta)} \quad \boxed{f_2(\theta)} \quad \boxed{f_s(\theta)} \\ | \quad | \quad | \\ \text{---} \quad \text{---} \quad \text{---} \end{array} + \begin{array}{c} \pi \quad \pi \quad \pi \\ | \quad | \quad | \\ \boxed{f'_1(\theta)} \quad \boxed{f'_2(\theta)} \quad \boxed{f'_s(\theta)} \\ | \quad | \quad | \\ \boxed{f_1(\theta)} \quad \boxed{f_2(\theta)} \quad \boxed{f_s(\theta)} \\ | \quad | \quad | \\ \text{---} \quad \text{---} \quad \text{---} \end{array} + \dots + \begin{array}{c} \pi \quad \pi \quad \pi \\ | \quad | \quad | \\ \boxed{f'_1(\theta)} \quad \boxed{f'_2(\theta)} \quad \boxed{f'_s(\theta)} \\ | \quad | \quad | \\ \boxed{f_1(\theta)} \quad \boxed{f_2(\theta)} \quad \boxed{f_s(\theta)} \\ | \quad | \quad | \\ \text{---} \quad \text{---} \quad \text{---} \end{array} \end{aligned}$$



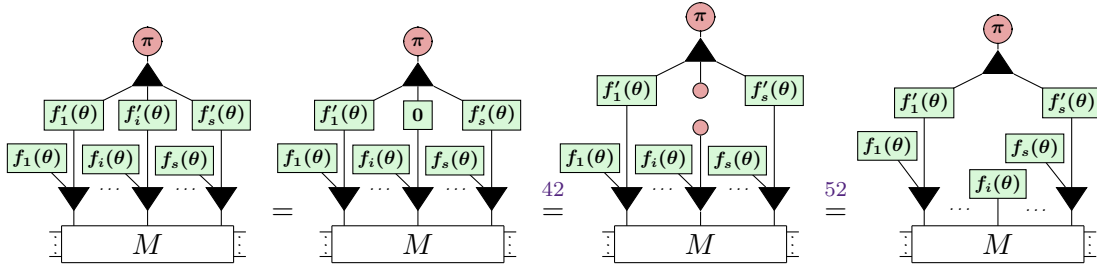
The first step follows from Lemma 13 and the product rule, the second step follows from Lemma 52 and Lemma 53, and the third step follows from the π commutation rule for green boxes. The final step uses the property of W spider as given in (1). $\square$

This theorem unifies the linearity and product rules of differential calculus into a single diagram, without a blowup in diagram size: the number of nodes added to the diagram after differentiation is linearly proportional to the number of parameter occurrences. This makes the result practically useful for both calculations by hand and computer simulation.

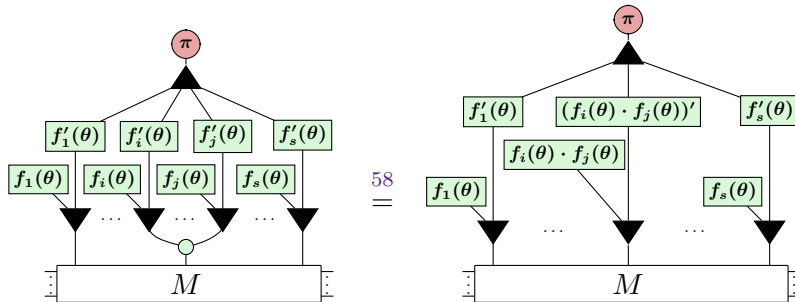
Remark 15. Using the chain rule, we can pull out a common factor if all f_i are composed with some other function g :



If f_i is a constant function, the corresponding spider does not contribute to the derivative:



Finally, the differentiation gadget nicely interacts with spider fusion:



Diagrammatic differentiation for regular ZX diagrams corresponds to the special case where all f_j are phase functions:

Theorem 16. *The derivative of a differentiable ZX diagram can be expressed as a single ZX diagram:*

$$\frac{\partial}{\partial \theta} \left[\begin{array}{c} g_1(\theta) \quad g_2(\theta) \quad \dots \quad g_s(\theta) \\ \vdots \\ M \\ \vdots \end{array} \right] = \begin{array}{c} \pi \\ \blacktriangle \\ \begin{array}{c} i \quad g'_1(\theta) \quad g'_2(\theta) \quad g'_s(\theta) \\ \pi \quad \downarrow \quad \downarrow \quad \downarrow \\ g_1(\theta) \quad g_2(\theta) \quad \dots \quad g_s(\theta) \\ \vdots \\ M \\ \vdots \end{array} \end{array}$$

Proof. This is a special case of Theorem 14, where $f_j(\theta) = e^{ig_j(\theta)} \neq 0$ and $\frac{f'_j(\theta)}{f_j(\theta)} = ig'_j(\theta)$, thus Lemma 57 applies. The “ i ” is common across all functions and can be factored out through the W spider using the diagrammatic chain rule from Remark 15. $\square$

Since we can now differentiate arbitrary ZX diagrams, we can consider differentiating quantum circuits as a special case of Theorem 16. Executing a circuit $U(\theta)$ for some observable H on a quantum computer estimates the expectation value $\langle H \rangle = \langle 0 | U^\dagger(\theta) H U(\theta) | 0 \rangle$. Thus, the ZX diagram representing $\langle H \rangle$ has an equal number of occurrences of θ and $-\theta$.

Corollary 17. *The derivative of a parameterised quantum circuit can be expressed as a single ZX diagram:*

$$\frac{\partial}{\partial \theta} \left[\begin{array}{c} \theta \quad \vdots \quad -\theta \\ \vdots \\ M \\ \vdots \end{array} \right] = \begin{array}{c} i \\ \pi \quad \blacktriangle \\ \begin{array}{c} \theta \quad \vdots \quad -\theta \\ \vdots \\ M \\ \vdots \end{array} \end{array}$$

Proof. Noting that $\frac{\partial}{\partial \theta} -\theta = -1$ and $\boxed{-1} = \pi$, this follows directly from Theorem 16. $\square$

Corollary 18. *As a special case of Corollary 17, we obtain the parameter-shift rule from [40].*

$$\frac{\partial}{\partial \theta} \left[\begin{array}{c} \theta \quad M \quad -\theta \end{array} \right] \stackrel{17}{=} \begin{array}{c} i \\ \pi \quad \blacktriangle \\ \begin{array}{c} \theta \quad M \quad -\theta \\ \vdots \end{array} \end{array} \stackrel{59}{=} \begin{array}{c} \pi \\ \begin{array}{c} \theta + \frac{\pi}{2} \quad M \quad -\theta - \frac{\pi}{2} \end{array} \end{array}$$

Remark 19. *This result has been given as a theorem in [52], here we directly get it as a consequence of Corollary 17 which follows from Theorem 16.*

From Corollary 17, we thus have a simple diagrammatic expression for the derivative of any parameterised quantum circuit. In general, it is not easy to obtain the derivative of a parameterised matrix in a single term bra-ket expression (with no sums, e.g. $\langle \phi | ABC | \psi \rangle$), thus showing the power of ZX-calculus and 2-dimensional diagrammatic reasoning.

Similar to how the decomposition of the Pauli X gate in Corollary 18 gives us a 2-term parameter shift rule, decompositions of the W state in Corollary 17 are used in [30] to obtain shift rules for gates with an arbitrary number of θ -occurrences in particular generalising the existing shift rules from [40] and [1]. Furthermore, they use the analytical ZX technology developed here to prove the optimality of the shift rule given in [1].

4 Integrating ZX diagrams

In this section we show how to diagrammatically integrate ZX diagrams using algebraic ZX-calculus. This will allow us to evaluate the expectation and variance of a quantum circuit's derivative over the uniform distribution, as demonstrated in Section 5.

4.1 Circuits

As a first step, we only consider integrals of diagrams with the same number of positive and negative occurrences of a parameter θ . In particular, all diagrams arising from expectation values of circuits have this form (see Section 5).

Definition 20. The Hamming weight of a bit-string $\vec{x} \in \{0, 1\}^n$ is defined as $w(\vec{x}) := \sum x_i$, i.e. the number of 1s in the bit-string.

Lemma 21. Let k be a non-zero integer and M a diagram with no occurrence of θ . Then

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \left(\begin{array}{c} n \\ \left\{ \begin{array}{c} k\theta \\ \vdots \\ k\theta \end{array} \right\} \\ m \\ \left\{ \begin{array}{c} \vdots \\ \vdots \end{array} \right\} \end{array} \right) M \left(\begin{array}{c} n \\ \left\{ \begin{array}{c} -k\theta \\ \vdots \\ -k\theta \end{array} \right\} \\ l \\ \left\{ \begin{array}{c} \vdots \\ \vdots \end{array} \right\} \end{array} \right) d\theta = \sum_{\substack{\vec{x}, \vec{y} \in \{0,1\}^n \\ w(\vec{x})=w(\vec{y})}} \left(\begin{array}{c} n \\ \left\{ \begin{array}{c} x_1\pi \\ \vdots \\ x_n\pi \end{array} \right\} \\ m \\ \left\{ \begin{array}{c} \vdots \\ \vdots \end{array} \right\} \end{array} \right) M \left(\begin{array}{c} n \\ \left\{ \begin{array}{c} y_1\pi \\ \vdots \\ y_n\pi \end{array} \right\} \\ l \\ \left\{ \begin{array}{c} \vdots \\ \vdots \end{array} \right\} \end{array} \right)$$

The diagram sum above has an exponential number of terms. We want to find a more compact representation of this integral as a single diagram. Since the common part M can be factored out of the sum, this is equivalent to finding a single diagram representation of the following projector.

Definition 22. The Hamming weight projector P_n is defined as

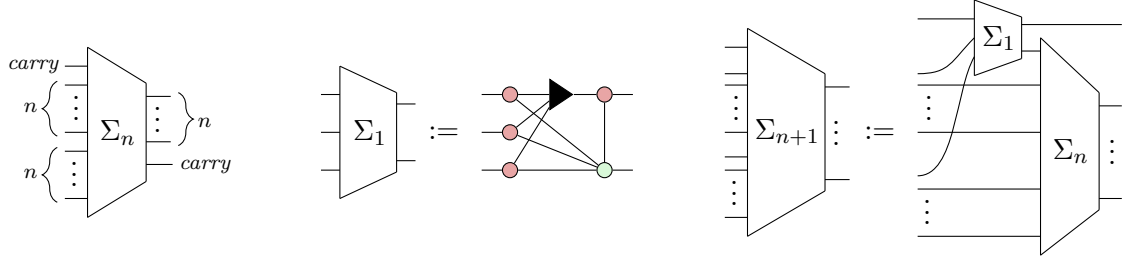
$$\left(\begin{array}{c} \vdots \\ P_n \\ \vdots \end{array} \right) := \sum_{\substack{\vec{x}, \vec{y} \in \{0,1\}^n \\ w(\vec{x})=w(\vec{y})}} \left(\begin{array}{c} \vdots \\ x_1\pi \\ \vdots \\ x_n\pi \end{array} \right) \left(\begin{array}{c} y_1\pi \\ \vdots \\ y_n\pi \end{array} \right)$$

We note that the Hamming weight of a bit-string of length n can be encoded in $\lfloor \log n \rfloor + 1$ bits using the standard binary encoding of natural numbers.

Definition 23. We write $[\vec{x}] := \sum_{i=1}^n 2^{i-1} x_i$ for the binary interpretation of a bit-string $\vec{x} \in \{0, 1\}^n$.

In the following, we use techniques from classical boolean circuits for binary arithmetic to construct an algebraic ZX diagram that outputs the Hamming weight in this encoding. We begin by giving a ZX analogue of a binary addition circuit for n bits.

Definition 24. We define the diagram Σ_n recursively via

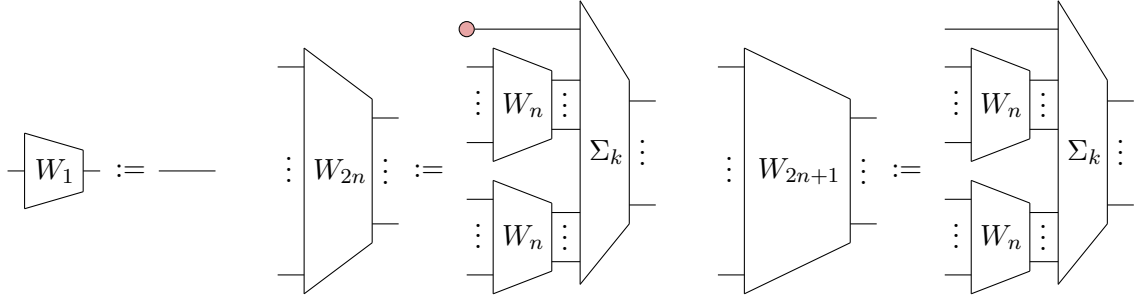


The construction of Σ_n is analogous to a classical ripple-carry adder, where Σ_1 acts as a full-adder [35]. Its action on computational basis states thus corresponds to binary addition.

Lemma 25. Σ_n performs binary addition, i.e. for all $\vec{x}, \vec{y} \in \{0, 1\}^n$ and $c \in \{0, 1\}$, we have $\Sigma_n |c, \vec{x}, \vec{y}\rangle = |\vec{z}\rangle$ where $[\vec{z}] = [\vec{x}] + [\vec{y}] + c$.

Using this adder, we define a diagram that computes the binary Hamming weight of its input using a divide-and-conquer strategy.

Definition 26. We define the diagram $n \left\{ \begin{array}{c} \vdots \\ W_n \\ \vdots \end{array} \right\}_{\lfloor \log n \rfloor + 1}$ recursively via



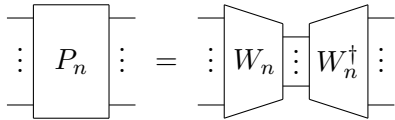
where $k = \lfloor \log n \rfloor + 1$.

Proposition 27. The diagram size of W_n only grows linearly with increasing n .

Lemma 28. W_n computes the binary Hamming weight, i.e. for all $\vec{x} \in \{0, 1\}^n$, we have $W_n |\vec{x}\rangle = |\vec{z}\rangle$ where $[\vec{z}] = w(\vec{x})$.

This immediately yields a single diagram representation of the Hamming weight projector P_n .

Corollary 29. We can represent P_n as a single diagram in terms of W_n :



Proof. Follows by comparing the action on all computational basis states. For all $\vec{x}, \vec{y} \in \{0, 1\}^n$, we have

$$\begin{array}{c} \text{red oval } x_1\pi \\ \vdots \\ \text{red oval } x_n\pi \end{array} \begin{array}{c} \vdots \\ P_n \\ \vdots \end{array} \begin{array}{c} \text{red oval } y_1\pi \\ \vdots \\ \text{red oval } y_n\pi \end{array} \stackrel{22}{=} \begin{cases} 1 & \text{if } w(\vec{x}) = w(\vec{y}) \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{array}{c}
\begin{array}{c} \textcircled{x_1 \pi} \\ \vdots \\ \textcircled{x_2 \pi} \end{array} \begin{array}{c} \diagdown \\ \vdots \\ \diagup \end{array} W_n \begin{array}{c} \diagup \\ \vdots \\ \diagdown \end{array} W_n^\dagger \begin{array}{c} \textcircled{y_1 \pi} \\ \vdots \\ \textcircled{y_n \pi} \end{array} \stackrel{28}{=} \begin{array}{c} \textcircled{a_1 \pi} \textcircled{b_1 \pi} \\ \vdots \\ \textcircled{a_k \pi} \textcircled{b_k \pi} \end{array} = \begin{cases} 1 & \text{if } \vec{a} = \vec{b} \\ 0 & \text{otherwise} \end{cases} = \begin{cases} 1 & \text{if } w(\vec{x}) = w(\vec{y}) \\ 0 & \text{otherwise} \end{cases}
\end{array}$$

where $k = \lfloor \log(n) \rfloor + 1$, $[\vec{a}] = w(\vec{x})$, and $[\vec{b}] = w(\vec{y})$. The last step follows since the binary interpretation $[\cdot]$ is a bijective mapping, so $\vec{a} = \vec{b} \iff [\vec{a}] = [\vec{b}] \iff w(\vec{x}) = w(\vec{y})$. $\square$

Theorem 30. Let k be a non-zero integer and M a diagram with no occurrence of θ . Then

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \left\{ \begin{array}{c} n \\ \vdots \\ k\theta \\ \vdots \\ k\theta \\ \vdots \end{array} \right\} M \left\{ \begin{array}{c} \vdots \\ -k\theta \\ \vdots \\ -k\theta \\ \vdots \end{array} \right\} d\theta = \begin{array}{c} \begin{array}{c} \vdots \\ W_n \\ \vdots \end{array} \begin{array}{c} \vdots \\ W_n^\dagger \\ \vdots \end{array} \\ \vdots \\ M \\ \vdots \end{array}$$

Proof. Immediately follows from Lemma 21 and Corollary 29. $\square$

Similar to the differentiation diagrams from the previous section, the size of this integration diagram is linear in n (follows from Proposition 27).

4.2 General Integration

Now, we can easily extend the integration result from circuits to arbitrary ZX diagrams with a different number of positive and negative occurrences of θ .

Theorem 31. Let k be a non-zero integer, M a diagram with no occurrence of θ , and w.l.o.g. $m \leq n$. Then

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \left\{ \begin{array}{c} n \\ \vdots \\ k\theta \\ \vdots \\ k\theta \\ \vdots \end{array} \right\} M \left\{ \begin{array}{c} \vdots \\ -k\theta \\ \vdots \\ -k\theta \\ \vdots \end{array} \right\} d\theta = \begin{array}{c} \begin{array}{c} \vdots \\ W_n \\ \vdots \end{array} \begin{array}{c} \vdots \\ W_n^\dagger \\ \vdots \end{array} \\ \vdots \\ M \\ \vdots \end{array}$$

Proof. We can rewrite the diagram into one with the same number of positive and negative occurrences of θ by exploiting the fact that $\textcircled{k\theta} \textcircled{\bullet} = \textcircled{-k\theta} \textcircled{\bullet} = 1$.

$$\left\{ \begin{array}{c} n \\ \vdots \\ k\theta \\ \vdots \\ k\theta \\ \vdots \end{array} \right\} M \left\{ \begin{array}{c} \vdots \\ -k\theta \\ \vdots \\ -k\theta \\ \vdots \end{array} \right\} = \left\{ \begin{array}{c} \vdots \\ k\theta \\ \vdots \\ k\theta \\ \vdots \end{array} \right\} M \left\{ \begin{array}{c} \vdots \\ -k\theta \\ \vdots \\ -k\theta \\ \vdots \end{array} \right\}$$

Then, the result immediately follows from Theorem 30. $\square$

4.3 Examples

To conclude, we explicitly give the integration diagrams for the cases $n = 1, 2, 3$ to illustrate and compare our integration approach with the work in [52].

Example 32. Let k be a non-zero integer and M a diagram with no occurrence of θ . Then

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \left\{ \begin{array}{c} k\theta \\ \vdots \\ -k\theta \end{array} \right\}_m \left\{ \begin{array}{c} -k\theta \\ \vdots \\ k\theta \end{array} \right\}_n d\alpha \stackrel{30}{=} \left\{ \begin{array}{c} \text{loop} \\ \vdots \\ M \\ \vdots \end{array} \right\}_n$$

This equation has been proved in [52] for $k = 1$. Here we obtain the result directly from Theorem 30 using the fact that W_1 is the identity.

Example 33. Let k be a non-zero integer and M a diagram with no occurrence of θ . Then

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \left\{ \begin{array}{c} k\theta \\ k\theta \\ \vdots \\ -k\theta \\ -k\theta \end{array} \right\}_m \left\{ \begin{array}{c} -k\theta \\ -k\theta \\ \vdots \\ k\theta \\ k\theta \end{array} \right\}_n d\theta \stackrel{30}{=} \left\{ \begin{array}{c} \text{loop with } m \text{ nodes} \\ \vdots \\ M \\ \vdots \end{array} \right\}_n \stackrel{67}{=} \left\{ \begin{array}{c} \text{loop with } m \text{ nodes and } n \text{ nodes} \\ \vdots \\ M \\ \vdots \end{array} \right\}_n$$

The corresponding result of this theorem is shown as Lemma 2 in [52] where there are three diagrammatic sum terms after integration, which results in their computation of variance of gradients becoming rather complicated. Here we only obtain a single diagram after integration.

Example 34. Let k be a non-zero integer and M a diagram with no occurrence of θ . Then

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \left\{ \begin{array}{c} k\theta \\ k\theta \\ k\theta \\ \vdots \\ -k\theta \\ -k\theta \\ -k\theta \end{array} \right\}_m \left\{ \begin{array}{c} -k\theta \\ -k\theta \\ -k\theta \\ \vdots \\ k\theta \\ k\theta \\ k\theta \end{array} \right\}_n d\theta \stackrel{30}{=} \left\{ \begin{array}{c} \text{loop with } m \text{ nodes} \\ \vdots \\ M \\ \vdots \end{array} \right\}_n$$

Zhao and Gao only considered diagrams with up to 2 occurrences of $\pm\theta$, so an equivalent result does not exist in [52].

5 Example Application: Quantum Machine Learning

In the NISQ era of quantum computing [39], many applications require the optimisation of parameterised quantum circuits: in quantum chemistry, variational quantum eigensolvers [33] are optimised to find the ground state of a Hamiltonian; in quantum machine learning, a circuit ansatz is optimised against a cost function [32], much alike how neural networks are optimised in classical machine learning.

However, while the approach of using gradient-based methods to optimise deep neural networks has been consistently effective [9], gradient-based optimisation of parameterised quantum circuits often suffer from barren plateaus: the training landscape of many circuit ansätze have been shown to be exponentially flat with respect to circuit size, making gradient descent impossible [37]. Therefore, it is crucial to develop techniques to detect and avoid barren plateaus.

So far, there has not been a fully diagrammatic analysis of barren plateaus using ZX-calculus. We believe the main obstacle to the analysis is the lack of techniques for manipulating sums of diagrams: an expectation of a Hamiltonian contains at least two occurrences of each circuit parameter, so the derivative of the expectation with respect to that parameter requires the product rule. Similarly, the rule for integrating diagrams in [52] introduces three terms, after n integrals there would be 3^n terms. Using these rules, the analysis of barren plateaus becomes exponentially costly, as the number of diagrams to be evaluated is exponential to the number of parameters in the circuit.

In this section, as a demonstration of the new differentiation and integration techniques of this paper, we show that the analysis of barren plateaus by Zhao et al. [52] can be done entirely within the framework of ZX without introducing sums of diagrams. Using the same setup, we consider an n -qubit parameterised quantum circuit $U(\theta)$ and a Hamiltonian H , obtaining the expectation value $\langle H \rangle = \langle 0 | U^\dagger(\theta) H U(\theta) | 0 \rangle$. If $\text{Var} \left(\frac{\partial \langle H \rangle}{\partial \theta_j} \right) \approx 0$ for all j , then the quantum circuit is likely to start in a barren plateau where the circuit gradients $\frac{\partial \langle H \rangle}{\partial \theta_j}$ are close to 0.

5.1 Method

Similar to Zhao et al. [52], we make some assumptions on the circuit $U(\theta)$:

1. The parameterised gates in U are R_X , R_Y , or R_Z and do not share parameters.
2. The parameters θ are independently and uniformly distributed on the interval $[\pi, -\pi]$.

This allows us to represent $U(\theta)$ as a ZX diagram where each parameter θ_j only occurs once. Thus, we can use the following notation for the expectation value $\langle H \rangle = \langle 0 | U^\dagger(\theta) H U(\theta) | 0 \rangle$ where the parametrised spiders are fused out.

$$\langle H \rangle = \begin{array}{c} \textcircled{\theta_1} \\ \vdots \\ \textcircled{\theta_m} \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \begin{array}{c} \textcircled{-\theta_1} \\ \vdots \\ \textcircled{-\theta_m} \end{array} \quad (2)$$

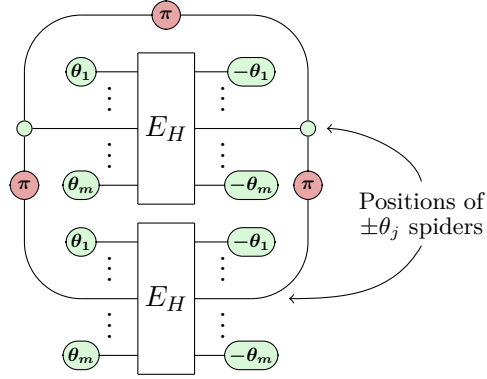
Lemma 35. [52] *Given $\langle H \rangle$ in the form of (2), we have $\mathbf{E} \left(\frac{\partial \langle H \rangle}{\partial \theta_j} \right) = 0$, for $j = 1, \dots, m$.*

As a consequence, we have

$$\begin{aligned} \text{Var} \left(\frac{\partial \langle H \rangle}{\partial \theta_j} \right) &= \mathbf{E} \left(\left(\frac{\partial \langle H \rangle}{\partial \theta_j} \right)^2 \right) \\ &= \frac{1}{(2\pi)^m} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \left(\frac{\partial \langle H \rangle}{\partial \theta_j} \right)^2 d\theta_1 \cdots d\theta_m, j = 1, \dots, m. \end{aligned}$$

Note that we can use squares here since the expectation value $\langle H \rangle$ is a real variable.

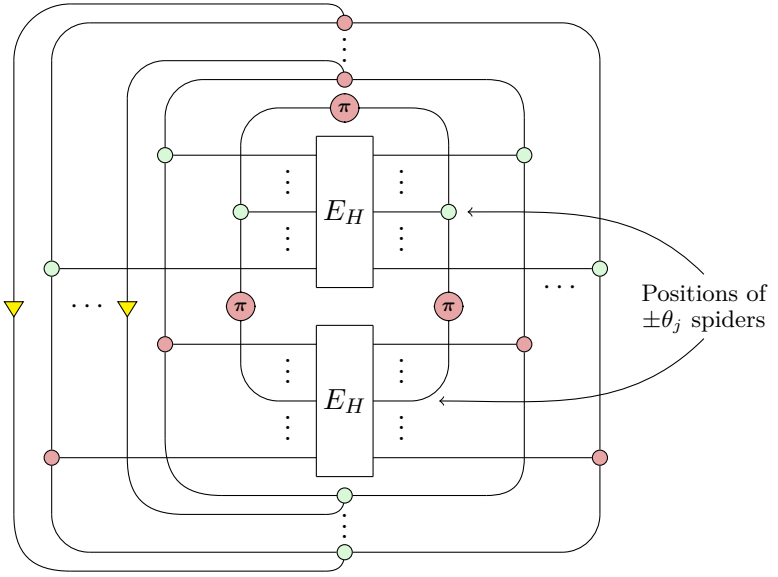
Lemma 36. [52] Given $\langle H \rangle$ in the form of (2), we have

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \left(\frac{\partial \langle H \rangle}{\partial \theta_j} \right)^2 d\theta_j =$$


where the cycle connects the legs of E_H that correspond to the positions of the $\pm\theta_j$ spiders in (2).

Remark 37. An equivalent version of this lemma is given on page 12 in [52]. Here, we obtain the result using our general differentiation and integration method.

Theorem 38. Given $\langle H \rangle$ in the form of (2), we have

$$\text{Var} \left(\frac{\partial \langle H \rangle}{\partial \theta_j} \right) =$$


Proof. We start from the diagram as shown in Lemma 36, then drag out variables iteratively according to Example 33, and the result follows. $\square$

Remark 39. The variance computed in [52] is based on a sum over 3^{m-1} terms (m is the number of parameters in the considered circuit), so when m is large it becomes infeasible to analyse the variance purely within ZX. Thus they have to resort to tensor networks which goes beyond the ZX method. In contrast, we avoid this exponential explosion by integrating without sums using algebraic ZX-calculus.

5.2 Example

Finally, we demonstrate Theorem 38 by analysing an example ansatz for the existence of barren plateaus. Concretely, we study the following n -qubit hardware efficient ansatz from [42], which

to the best of our knowledge has not been analysed before.

Figure 1 illustrates the quantum circuit for the generalized GHZ state. The circuit consists of \$n\$ qubits. Each qubit starts with a Hadamard (\$H\$) gate. The first \$n-1\$ qubits are then entangled with the \$n\$th qubit using a series of controlled operations. The final state is a generalized GHZ state, which can be written as:

$$\frac{1}{\sqrt{2^{n-1}}} \sum_{j=0}^{2^{n-1}-1} \exp(i j \theta_1) \exp(i j \theta_2) \dots \exp(i j \theta_n) |j\rangle$$

Here, we used the standard ZX representation of quantum gates, i.e.

$$H = \text{---} \text{---} \text{---}, \quad R_X(\theta) = \text{---} \text{---} \text{---}, \quad CZ = \text{---} \text{---} \text{---}$$

and we used blue dashed lines  to denote wires  with a Hadamard gate on them. For this example, we will consider the Hamiltonian $H = Z^{\otimes n}$ which corresponds to measuring all qubits in the computational basis. This gives us

Figure 1 shows three quantum circuit diagrams. The first diagram, labeled $\langle H \rangle =$, shows a sequence of n terms. Each term consists of a green circle labeled θ_i , a red circle labeled π , and a green circle labeled $-\theta_i$, all connected by blue dashed lines. A red circle labeled 2^{n-1} is at the top. The second diagram, labeled $\equiv$, shows the same sequence of terms, but the red circle is labeled $\frac{1}{2}$. The third diagram, labeled $=$, shows the same sequence of terms, but the red circle is labeled $\frac{1}{2}$ and the entire sequence is enclosed in a dashed box labeled E_H .

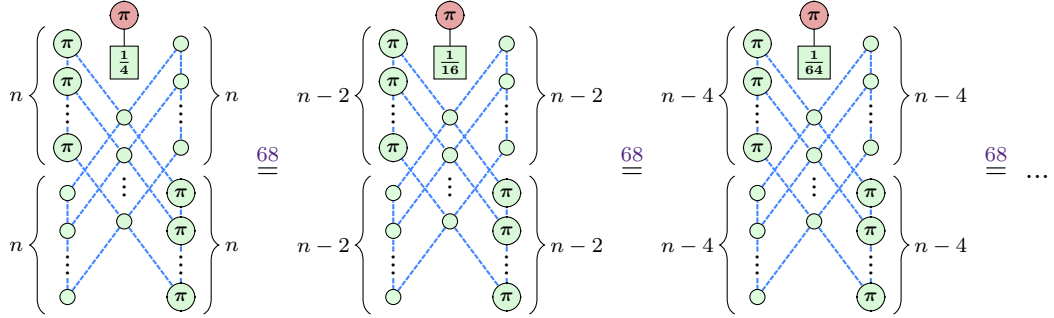
Now, we can use Theorem 38 to get a single ZX diagram that represents the variance of $\langle H \rangle$'s gradient w.r.t. some parameter θ_j .

Diagram (3) illustrates a quantum circuit for the variance of the derivative of the expectation value of H with respect to θ_j . The circuit starts with a red circle containing π and a green square containing $\frac{1}{4}$. It then branches into multiple paths, each containing a series of green circles connected by dashed blue lines, with red circles containing π interspersed. The paths are connected by solid black lines, and the circuit ends with a yellow triangle. A label "Positions of $\pm\theta_j$ spiders" points to the green circles.

Lemma 40. *The cycles in diagram (3) can be broken up as follows.*

Proposition 41. *The ansatz $U(\theta)$ suffers from barren plateaus for $H = Z^{\otimes n}$.*

Proof. Using Lemma 40, we simplify the variance diagram (3) to



The initial diagram contains $5n$ spiders connected by Hadamard edges. We repeatedly apply Lemma 68, each time reducing the number of spiders by 10 and collecting a scalar of $\frac{1}{4}$. Depending on the parity of n , we will end up with 5 or 10 spiders scaled by $\frac{1}{2^n}$. Since the final diagram size is constant in n , we can conclude that the overall scaling is in $O\left(\frac{1}{2^n}\right)$. Thus, $U(\theta)$ suffers from barren plateaus. $\square$

Our diagrammatic differentiation and integration approach allowed us to carry out this analysis purely using simple reasoning and rewriting on polynomially-sized ZX diagrams. Compared to Zhao et al. [52], we did not need to resort to general tensor networks or consider diagrams with an exponential number of terms or exponential size.

For more advanced examples of barren plateau detection using Theorem 38 we refer to [30] where more ansätze from [42] as well as IQP ansätze [41] are analysed using our approach.

6 Conclusion and further work

We have elevated ZX-calculus from a graphical language for algebraic calculations to a new graphical tool for analytical reasoning. For example, it can now be used for tackling quantum optimisation problems and reasoning about quantum mechanics. We believe these techniques will extend the applicability of ZX-calculus to more problems related to quantum computing. With more work, ZX-calculus can become a general tool for graphical differential calculus.

There are many directions for future work:

1. **Generalisation of the results to qudit and qufinite cases [50]:** The ideas in this paper can be extended beyond qubits, giving us more diagrammatic analytical tools.
2. **Indefinite integration:** This paper only gives the definite integral for ZX diagrams between $\pm\pi$. Indefinite integration of arbitrary ZX diagrams would in a sense complete the analytical ZX-calculus.
3. **Parameter shift rules:** As pointed out in Corollary 18, we recovered a graphical version of the parameter shift rule from [40]. Our diagrammatic approach might prove useful to discover more general shift rules or other gradient computation methods. See [30] for some initial investigations in this area.
4. **Numerical barren plateau detection:** Since the diagram in Theorem 38 is mostly Clifford, we can use stabiliser decomposition methods [28, 29] to evaluate it. As shown in [31], this allows us to numerically detect barren plateaus more efficiently than previous sampling-based methods.

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A Proofs and Lemmas

In this appendix, we include all the lemmas with their proofs which have been essentially existed (up to scalars) in previous papers. The lemmas are given in the order which they appear in this paper.

Lemma 10.

Proof.

□

Lemma 11. Suppose $f(\theta)$ is a differentiable real function of θ . Then

Proof.

□

Lemma 12. For any complex number a , we have

Proof.

□

Lemma 13. Suppose $f : \mathbb{R} \rightarrow \mathbb{C}$ is a differentiable function. Then

Proof.

□

Lemma 42.

Proof.

□

Lemma 43.

Proof.

$$\begin{aligned}
 & \begin{array}{c} n \\ \vdots \\ \text{---} \\ \vdots \\ m \end{array} X = \begin{array}{c} \pi \\ \vdots \\ \frac{n+m-2}{2} \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} \stackrel{Z}{=} \begin{array}{c} \pi \\ \vdots \\ \frac{n+m-2}{2} \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} + \begin{array}{c} \pi \\ \vdots \\ \frac{n+m-2}{2} \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} \\
 & \stackrel{H2}{=} \begin{array}{c} \pi \\ \vdots \\ \frac{1}{2} \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} + \begin{array}{c} \pi \\ \vdots \\ \frac{1}{2} \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array}
 \end{aligned}$$

□

Lemma 44.

$$\begin{array}{c} \text{---} \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \text{---} \end{array}$$

Proof.

$$\begin{array}{c} \text{---} \\ \text{---} \end{array} \stackrel{3}{=} \begin{array}{c} \pi \\ \text{---} \\ \pi \end{array} \stackrel{Bas1}{=} \begin{array}{c} \pi \\ \text{---} \\ \pi \end{array} \stackrel{B1}{=} \begin{array}{c} \text{---} \\ \text{---} \end{array}$$

□

Lemma 45.

$$\begin{array}{c} \text{---} \\ \pi \end{array} = \begin{array}{c} \text{---} \\ \pi \end{array}$$

Proof.

$$\begin{array}{c} \text{---} \\ \pi \end{array} \stackrel{3}{=} \begin{array}{c} \pi \\ \text{---} \\ \pi \end{array} \stackrel{Bas0}{=} \begin{array}{c} \pi \\ \text{---} \\ \pi \end{array} \stackrel{S1r}{=} \begin{array}{c} \text{---} \\ \pi \end{array}$$

□

Lemma 46.

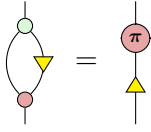
$$\begin{array}{c} \text{---} \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \text{---} \end{array}$$

Proof.

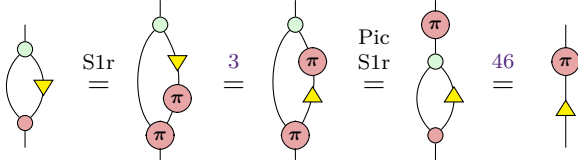
$$\begin{array}{c} \text{---} \\ \text{---} \end{array} \stackrel{S1}{=} \begin{array}{c} \text{---} \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \text{---} \end{array} \stackrel{Sym}{=} \begin{array}{c} \text{---} \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \text{---} \end{array} \stackrel{B1}{=} \begin{array}{c} \text{---} \\ \text{---} \end{array} \stackrel{S1}{=} \begin{array}{c} \text{---} \\ \text{---} \end{array} \stackrel{S2}{=} \begin{array}{c} \text{---} \\ \text{---} \end{array}$$

□

Lemma 47.

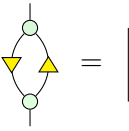


Proof.

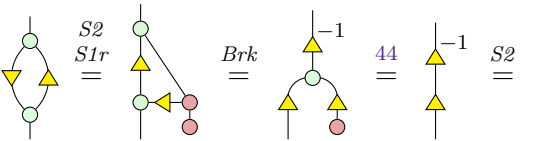


□

Lemma 48.

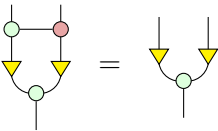


Proof.

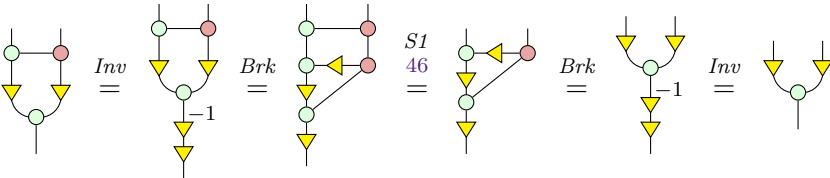


□

Lemma 49.

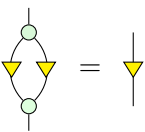


Proof.

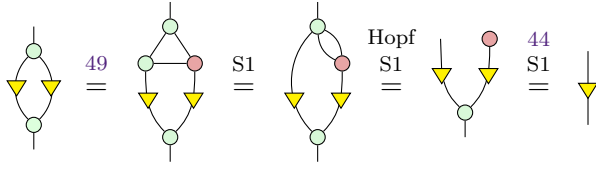


□

Lemma 50.

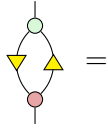


Proof.

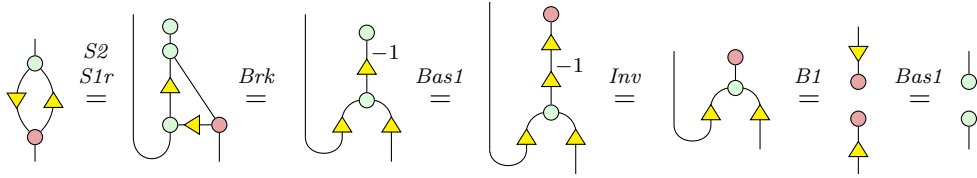


□

Lemma 51.

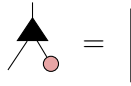


Proof.

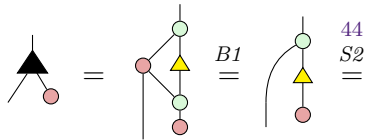


□

Lemma 52.

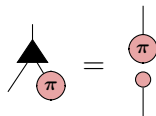


Proof.

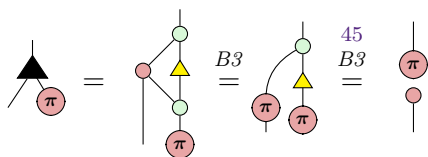


□

Lemma 53.



Proof.



□

Lemma 54.

Proof.

□

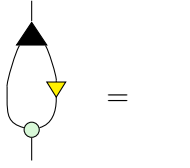
Lemma 55. Let $a, b \in \mathbb{C}$. Then

Proof. If $b = 0$, then

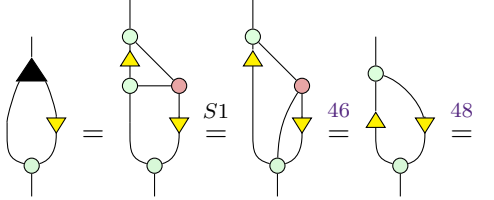
If $b \neq 0$, then

□

Lemma 56.

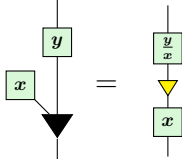


Proof.

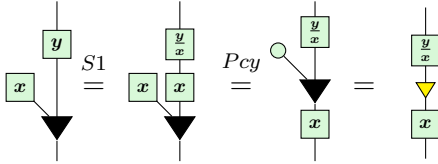


□

Lemma 57. Let $0 \neq x, y \in \mathbb{C}$. Then

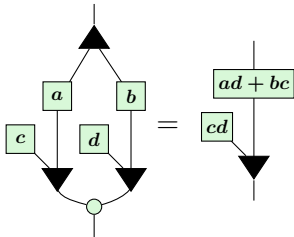


Proof.

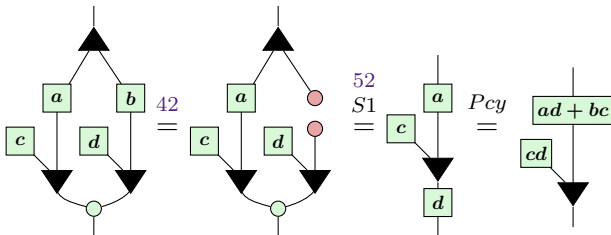


□

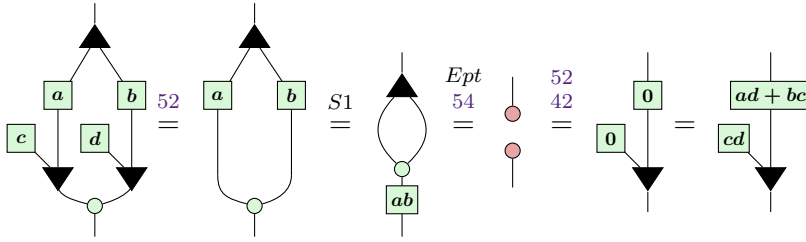
Lemma 58. Let $a, b, c, d \in \mathbb{C}$. Then



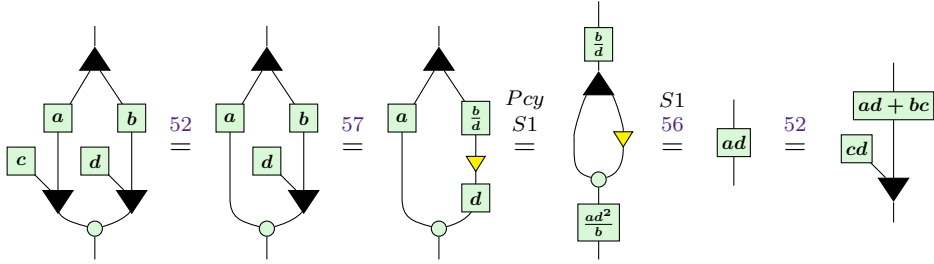
Proof. If $b = 0$, then



If $b \neq 0, c = d = 0$, then



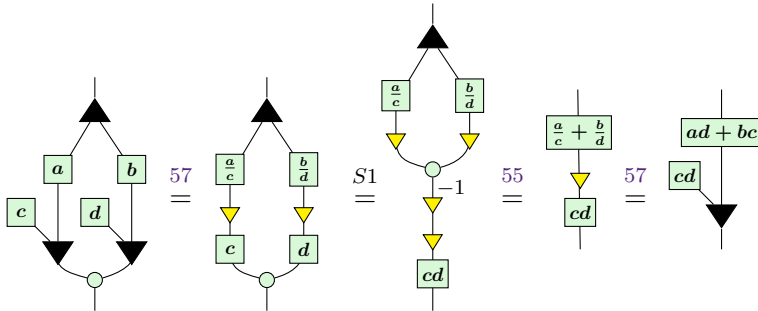
If $b \neq 0, c = 0, d \neq 0$, then



If $b \neq 0, c \neq 0, a = 0$, then the proof is similar to the case when $b = 0$.

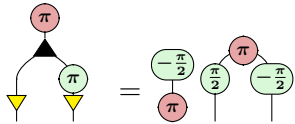
If $b \neq 0, c \neq 0, a \neq 0, d = 0$, then the proof is similar to the case when $b \neq 0, c = 0, d \neq 0$.

If $b \neq 0, c \neq 0, a \neq 0, d \neq 0$, then

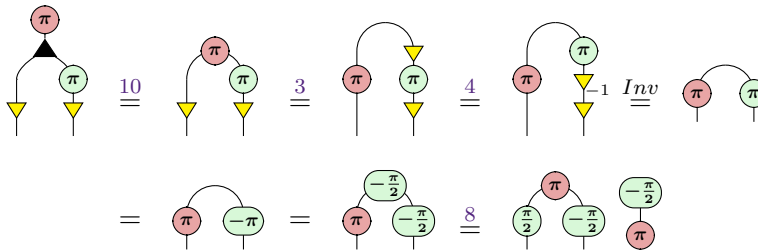


□

Lemma 59.

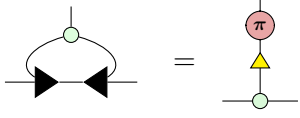


Proof.

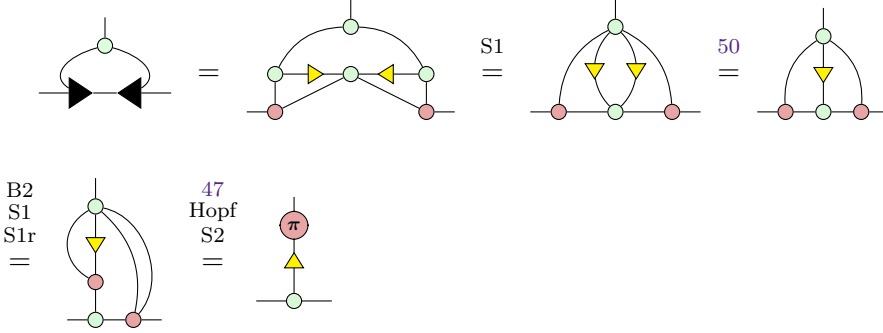


□

Lemma 60.

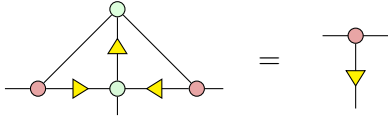


Proof.

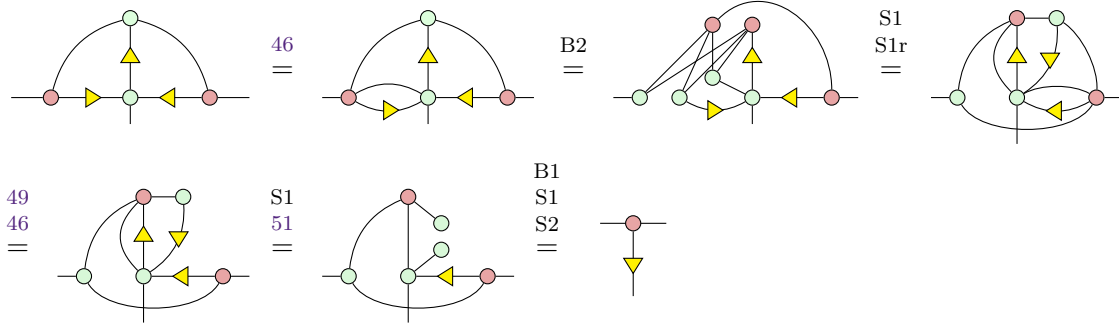


□

Lemma 61.



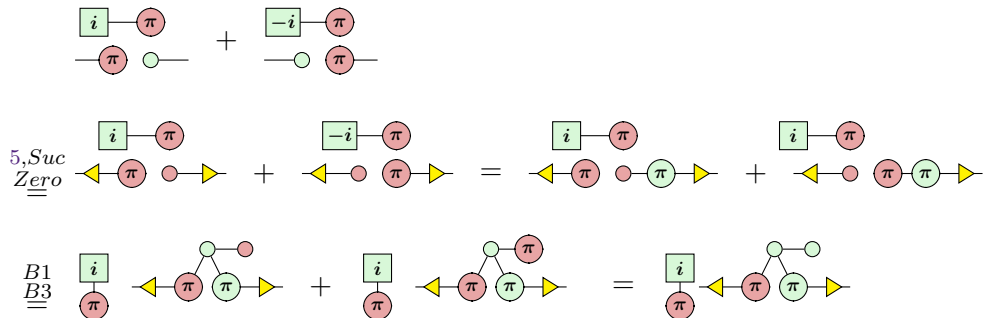
Proof.



□

Lemma 62. $\begin{array}{c} \boxed{i} \\ \pi \end{array} \begin{array}{c} \pi \\ \pi \end{array} + \begin{array}{c} \boxed{-i} \\ \pi \end{array} \begin{array}{c} \pi \\ \pi \end{array} = \begin{array}{c} \frac{\pi}{2} \\ \pi \end{array} \begin{array}{c} \pi \\ \pi \end{array} \begin{array}{c} -\frac{\pi}{2} \\ \pi \end{array}$

Proof. We use the triangle to do the change of basis from $|+\rangle$ and $|1\rangle$ to $|0\rangle$ and $|1\rangle$.



The rest of the proof is identical to the proof of Lemma 59. $\square$

Lemma 63.

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

Proof.

$$\text{Diagram 1} \stackrel{S1}{=} \text{Diagram 3} \stackrel{Hopf}{=} \text{Diagram 4} \stackrel{S1r}{\stackrel{S2}{=}} \text{Diagram 2}$$

$\square$

Lemma 64.

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

Proof.

$$\text{Diagram 1} \stackrel{S1}{=} \text{Diagram 3} \stackrel{Pic}{=} \text{Diagram 4} \stackrel{S1}{=} \text{Diagram 5} \stackrel{Hopf}{=} \text{Diagram 2}$$

$\square$

Lemma 65.

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

Proof.

$$\text{Diagram 1} \stackrel{S1}{=} \text{Diagram 3} \stackrel{Pic}{=} \text{Diagram 4} \stackrel{S1}{=} \text{Diagram 2}$$

$\square$

B Integration proofs

Lemma 21. Let k be a non-zero integer and M a diagram with no occurrence of θ . Then

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \left\{ \begin{array}{c} n \\ \vdots \\ k\theta \\ \vdots \\ k\theta \\ \vdots \\ m \end{array} \right\} M \left\{ \begin{array}{c} \vdots \\ -k\theta \\ \vdots \\ -k\theta \\ \vdots \\ l \end{array} \right\} d\theta = \sum_{\substack{\vec{x}, \vec{y} \in \{0,1\}^n \\ w(\vec{x})=w(\vec{y})}} \left\{ \begin{array}{c} x_1\pi \\ \vdots \\ x_n\pi \\ \vdots \\ m \end{array} \right\} M \left\{ \begin{array}{c} y_1\pi \\ \vdots \\ y_n\pi \\ \vdots \\ l \end{array} \right\}$$

Proof. We have

$$\textcircled{k\theta} \text{---} \stackrel{(Z)}{=} \textcircled{\cdot} \text{---} + e^{ik\theta} \textcircled{\pi} \text{---} = \sum_{x \in \{0,1\}} e^{ik\theta x} \textcircled{x\pi} \text{---} \quad (4)$$

Thus, we can decompose our diagram as follows:

$$\begin{aligned} & \begin{array}{c} \textcircled{k\theta} \text{---} \\ \vdots \\ \textcircled{k\theta} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \textcircled{-k\theta} \\ \vdots \\ \textcircled{-k\theta} \\ \vdots \end{array} \stackrel{(4)}{=} \sum_{\vec{x} \in \{0,1\}^n} e^{ik\theta w(\vec{x})} \begin{array}{c} \textcircled{x_1\pi} \text{---} \\ \vdots \\ \textcircled{x_n\pi} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \textcircled{-k\theta} \\ \vdots \\ \textcircled{-k\theta} \\ \vdots \end{array} \\ & \stackrel{(4)}{=} \sum_{\vec{x}, \vec{y} \in \{0,1\}^n} e^{ik\theta(w(\vec{x})-w(\vec{y}))} \begin{array}{c} \textcircled{x_1\pi} \text{---} \\ \vdots \\ \textcircled{x_n\pi} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \textcircled{y_1\pi} \\ \vdots \\ \textcircled{y_n\pi} \\ \vdots \end{array} \quad (5) \end{aligned}$$

Furthermore, for every integer $a \in \mathbb{Z}$, we have

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ia\theta} d\theta = \begin{cases} 1 & \text{if } a = 0 \\ \frac{2 \sin(a\pi)}{a} = 0 & \text{if } a \neq 0 \end{cases} \quad (6)$$

Therefore, we can conclude

$$\begin{aligned} & \frac{1}{2\pi} \int_{-\pi}^{\pi} \begin{array}{c} \textcircled{k\theta} \text{---} \\ \vdots \\ \textcircled{k\theta} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \textcircled{-k\theta} \\ \vdots \\ \textcircled{-k\theta} \\ \vdots \end{array} d\theta \stackrel{(5)}{=} \sum_{\vec{x}, \vec{y} \in \{0,1\}^n} \left(\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ik\theta(w(\vec{x})-w(\vec{y}))} d\theta \right) \begin{array}{c} \textcircled{x_1\pi} \text{---} \\ \vdots \\ \textcircled{x_n\pi} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \textcircled{y_1\pi} \\ \vdots \\ \textcircled{y_n\pi} \\ \vdots \end{array} \\ & \stackrel{(6)}{=} \sum_{\substack{\vec{x}, \vec{y} \in \{0,1\}^n \\ w(\vec{x})=w(\vec{y})}} \begin{array}{c} \textcircled{x_1\pi} \text{---} \\ \vdots \\ \textcircled{x_n\pi} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \end{array} \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \\ \vdots \end{array} \begin{array}{c} \textcircled{y_1\pi} \\ \vdots \\ \textcircled{y_n\pi} \\ \vdots \end{array} \end{aligned}$$

□

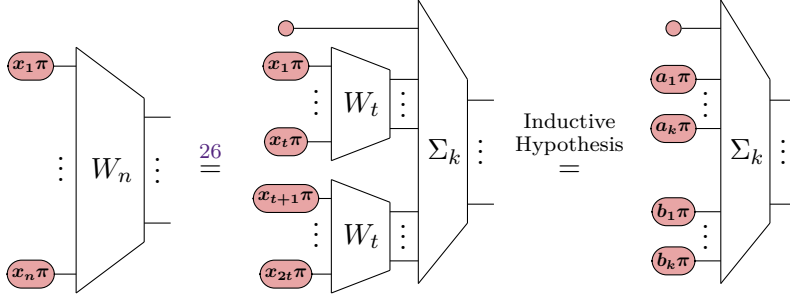
Lemma 66. Σ_1 is symmetric:

$$\begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} \Sigma_1 \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} \Sigma_1 \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} \Sigma_1 \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array} \Sigma_1 \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \end{array}$$

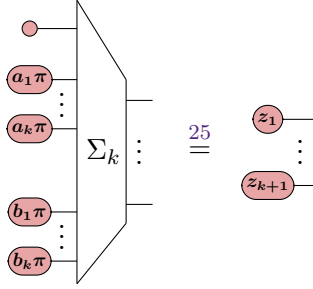
Proof. Immediately follows from the definition of Σ_1 and (Sym). □

Lemma 25. Σ_n performs binary addition, i.e. for all $\vec{x}, \vec{y} \in \{0,1\}^n$ and $c \in \{0,1\}$, we have $\Sigma_n |c, \vec{x}, \vec{y}\rangle = |\vec{z}\rangle$ where $[\vec{z}] = [\vec{x}] + [\vec{y}] + c$.

$n = 2t$ for some $t < n$, then



where $k = \lfloor \log(t) \rfloor + 1$, $[\vec{a}] = w(x_1, \dots, x_t)$, and $[\vec{b}] = w(x_{t+1}, \dots, x_{2t})$. Then



where $[\vec{z}] = [\vec{a}] + [\vec{b}] + 0 = w(x_1, \dots, x_t) + w(x_{t+1}, \dots, x_{2t}) = w(\vec{x})$ as required.

The case where n is odd follows similarly. $\square$

Proposition 27. *The diagram size of W_n only grows linearly with increasing n .*

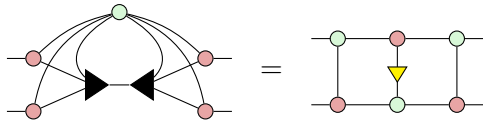
Proof. We denote the size of a ZX diagram D as $S(D)$. In the following, we only consider the size in big-O notation.

Clearly, we have $S(\Sigma_n) \in O(n)$. Following the definition of W_n , we thus have

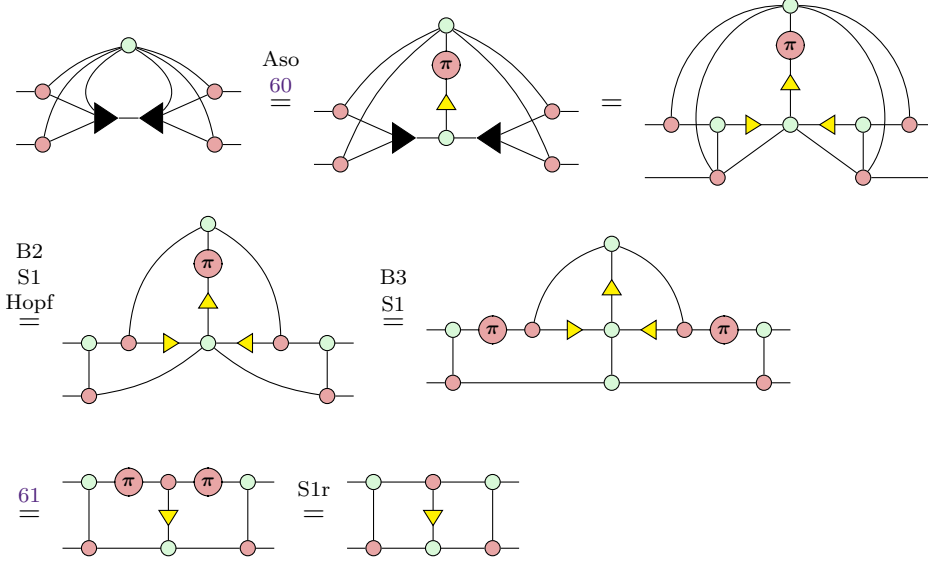
$$\begin{aligned} S(W_1) &= O(1), & S(W_n) &= 2S(W_{n/2}) + S(\Sigma_{\lfloor \log n \rfloor + 1}) && \text{for } n > 1 \\ & & &= 2S(W_{n/2}) + O(\lfloor \log n \rfloor + 1) \end{aligned}$$

The Master theorem [7] implies that this recurrence relation satisfies $S(W_n) \in O(n)$. $\square$

Lemma 67.



Proof.



□

C Barren Plateau Analysis

Lemma 35. [52] Given $\langle H \rangle$ in the form of (2), we have $\mathbf{E} \left(\frac{\partial \langle H \rangle}{\partial \theta_j} \right) = 0$, for $j = 1, \dots, m$.

Proof. By integrating over the uniform distribution, we have

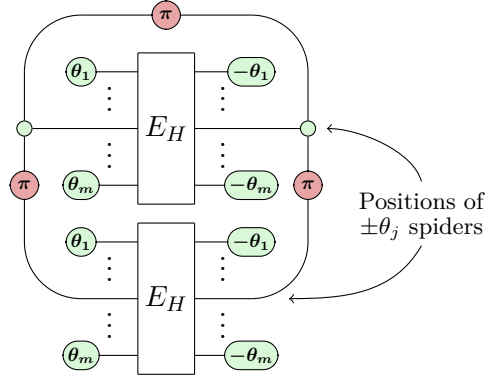
$$\mathbf{E} \left(\frac{\partial \langle H \rangle}{\partial \theta_j} \right) = \frac{1}{(2\pi)^m} \int_{-\pi}^{\pi} \dots \int_{-\pi}^{\pi} \frac{\partial \langle H \rangle}{\partial \theta_j} d\theta_1 \dots d\theta_m.$$

We prove the theorem by showing that $\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\partial \langle H \rangle}{\partial \theta_j} d\theta_j = 0$.

$$\begin{aligned} \frac{\partial \langle H \rangle}{\partial \theta_j} &\stackrel{18}{=} \text{Diagram 1} \\ \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\partial \langle H \rangle}{\partial \theta_j} d\theta_j &\stackrel{32}{=} \text{Diagram 2} \\ &\stackrel{63}{=} \text{Diagram 3} = 0 \end{aligned}$$

Since the unconnected pink π spider is equal to the zero scalar, the entire diagram evaluates to zero. □

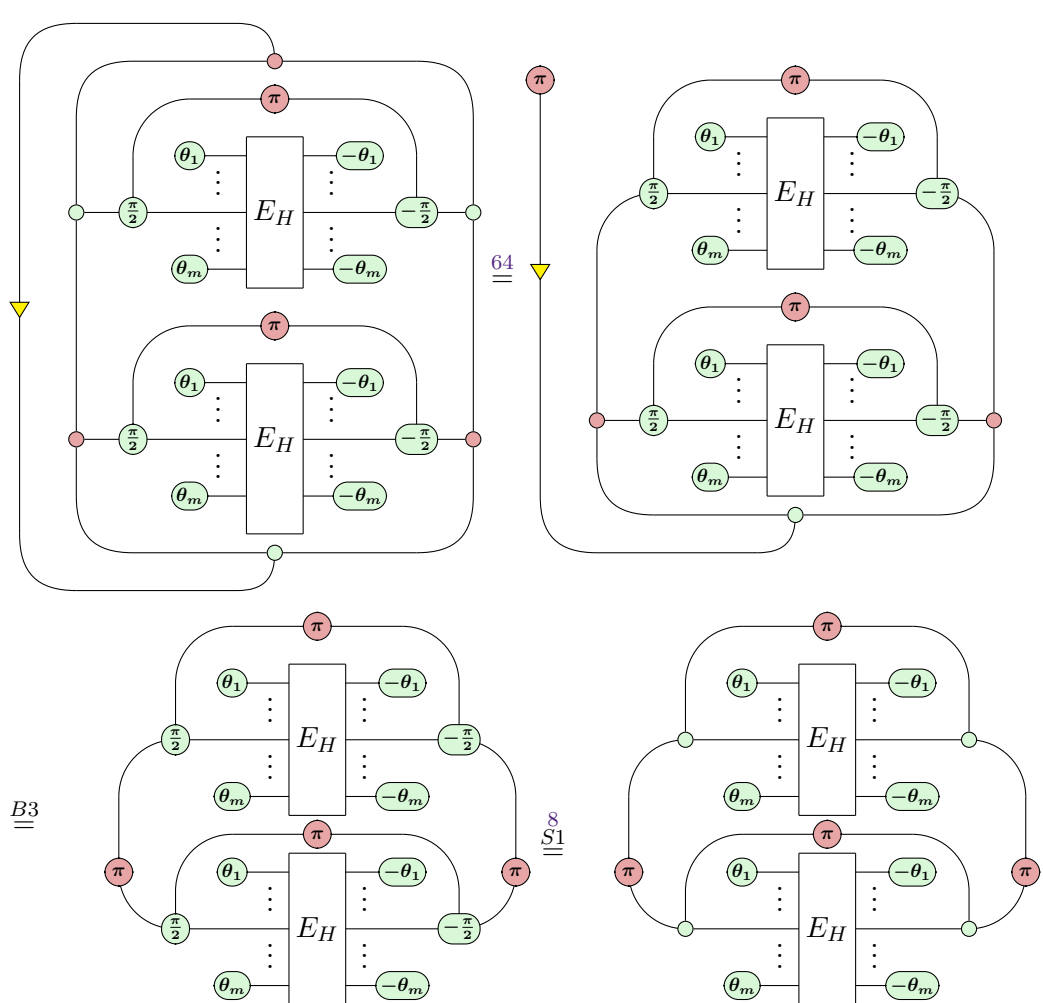
Lemma 36. [52] Given $\langle H \rangle$ in the form of (2), we have

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \left(\frac{\partial \langle H \rangle}{\partial \theta_j} \right)^2 d\theta_j =$$


Positions of $\pm\theta_j$ spiders

where the cycle connects the legs of E_H that correspond to the positions of the $\pm\theta_j$ spiders in (2).

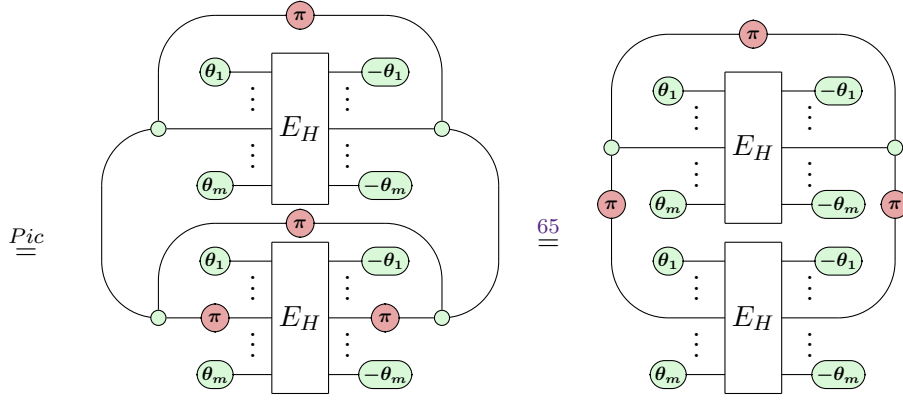
Proof. By Example 33,

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \left(\frac{\partial \langle H \rangle}{\partial \theta_j} \right)^2 d\theta_j =$$


64

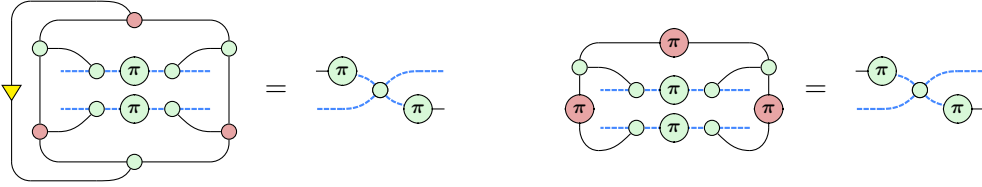
B3

S1

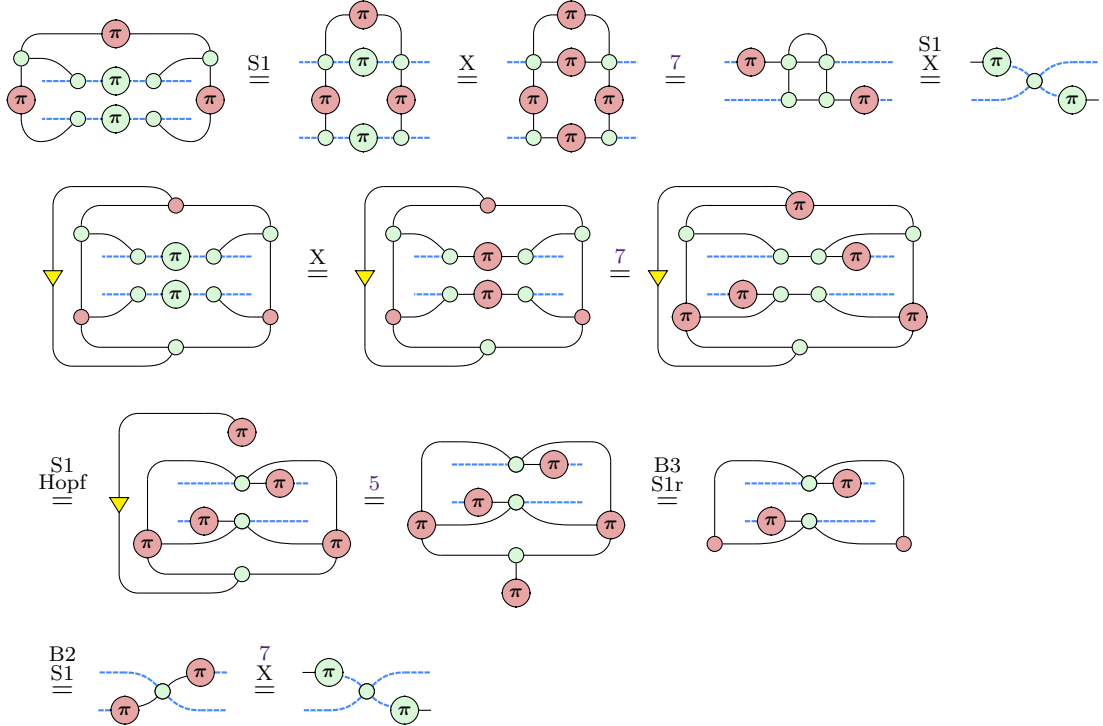


□

Lemma 40. *The cycles in diagram (3) can be broken up as follows.*

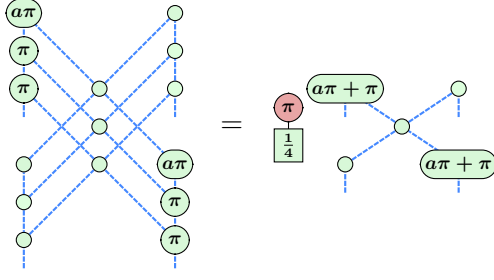


Proof.

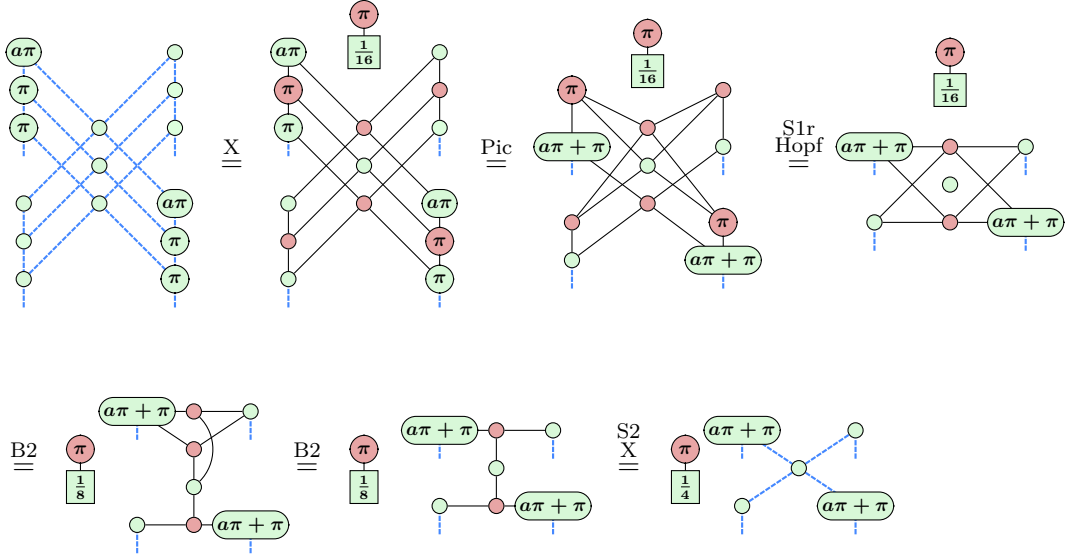


□

Lemma 68. For all $a \in \{0, 1\}$, we have



Proof.



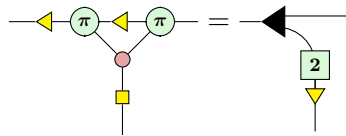
□

D Comparison with Jeandel et al.

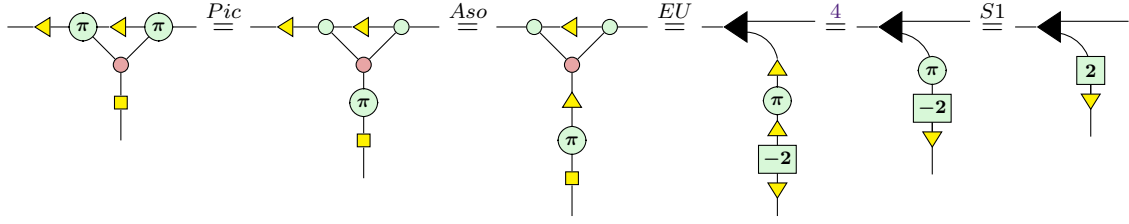
Jeandel, Perdrix, and Veshchezerova present an alternate method to represent derivatives with the ZX-calculus [24]. We want to show that the two papers arrive at similar results through very different techniques, and that some results in [24] can be more compactly represented by explicitly using the W spider. The nodes used in [24] are similar to ours: the circle green nodes, the Hadamard node and the red nodes are exactly the same, but we additionally have pink nodes which are different to the red nodes up to a variational scalar, and have green box nodes which have the circle green nodes as special cases while can be turned into circle green nodes with the help of the yellow triangle node [23]. Also note that their black triangle corresponds to our yellow triangle and our black triangle corresponds to the W spider.

First, we show that the triangular-shaped diagram that features in their differentiation result can be represented compactly using the W spider:

Lemma 69.

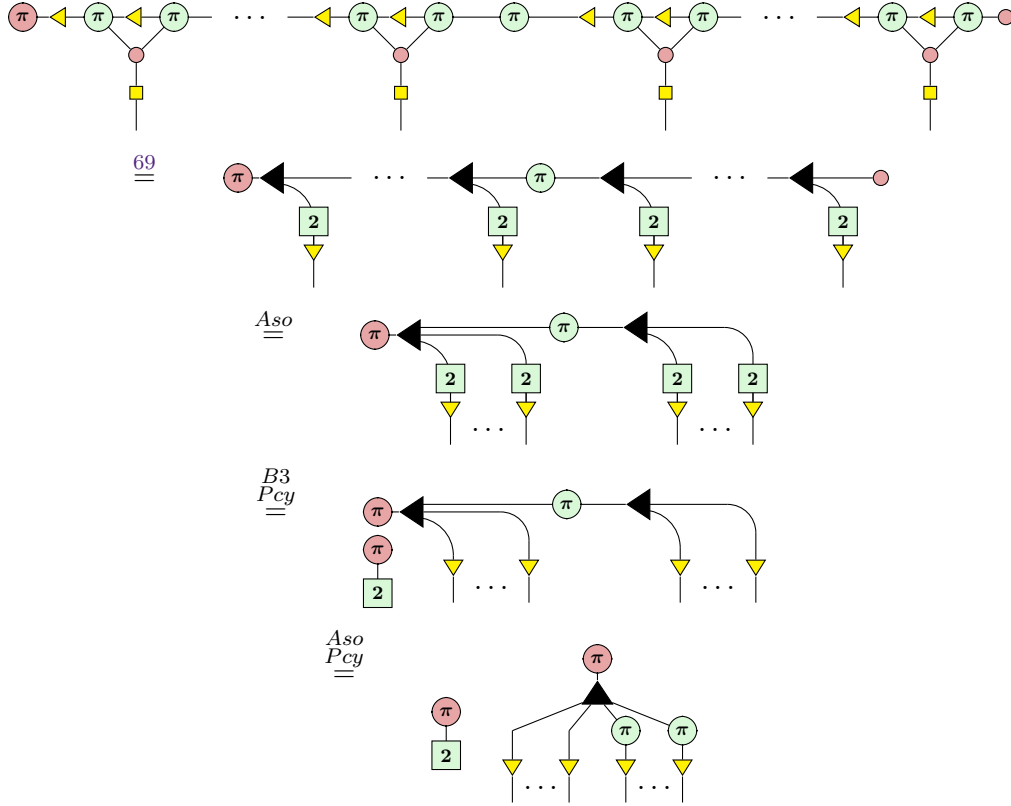


Proof.



□

Remark 70. The differentiation of “linear” ZX diagrams result obtained by [24] is equivalent to our lemma 17.



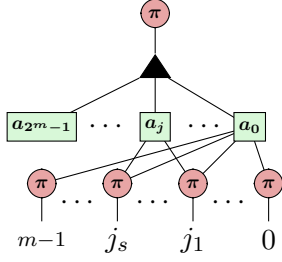
Although the end results are equivalent, we emphasise that their result is obtained through their theory of summing controlled diagrams, whilst our result is obtained through our arbitrary differentiation result.

Remark 71. The general differentiation result in [24] requires an inductive conversion to controlled diagrams, and is obtained through combining diagrammatic addition and the Leibniz product rule. Because of this, the resulting diagram will not resemble the original diagram.

In comparison, our Theorem 14 does not affect the topology of the original diagram and can be calculated almost instantly.

Remark 72. Both the general results on addition of diagrams and on differentiation of diagrams shown in [24] are based on induction on generators. If such induction methods

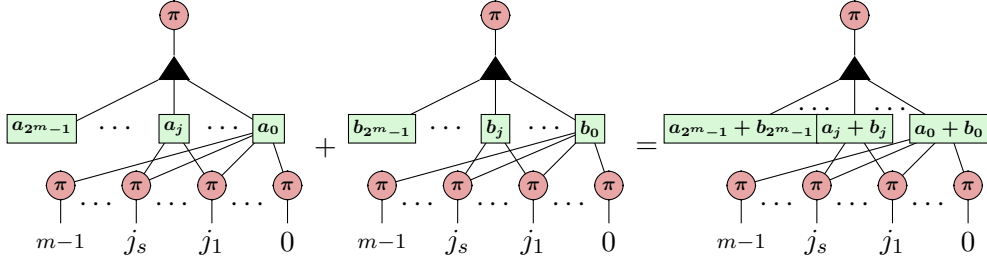
are allowed, then there is an alternative way to generally add two ZX diagrams or differentiate a ZX diagram: first rewrite inductively the diagrams into the compressed normal form shown in [48] as follows



which corresponding to the vector

$$\begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{2^m-2} \\ a_{2^m-1} \end{pmatrix},$$

then the sum of two diagrams can be obtained by adding up the corresponding parameters in the two diagrams:



and the differentiation can be obtained element-wisely:

