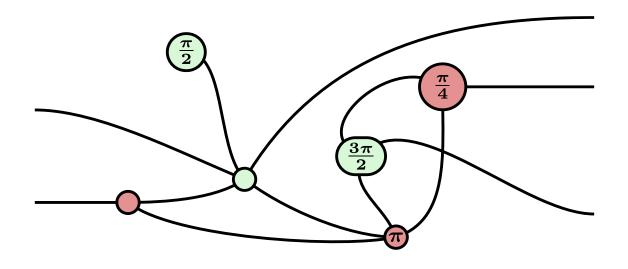


ZX-Calculus



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30.06.2023

What is ZX-Calculus?



- A graphical language extending circuit diagrams
 - Allows breaking up logic gates into smaller atoms
 - The resulting graph is a *low-level* representation of the circuit
- Using transformations on those atoms, we can visually deduce:
 - Properties of circuits
 - Entangled states
 - How quantum protocols work

<u>Applications</u>

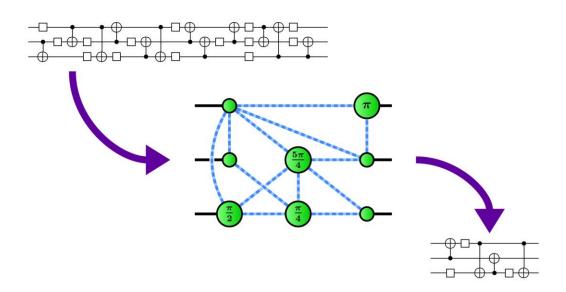


- Quantum circuit optimization
 - Reduce the complexity of circuits
 - T-count reduction
 - Important metric for performing fault-tolerant computations
- Circuit compilation
 - Reducing high-level quantum algorithms to run on a target architecture

Quantum Circuit optimization

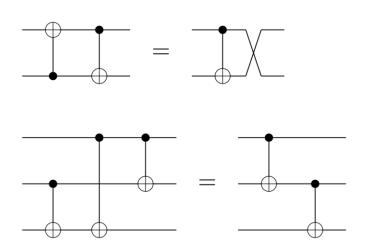


- Goal: Transform circuits into equivalent circuits
 - New Circuit must have fewer / simpler gates





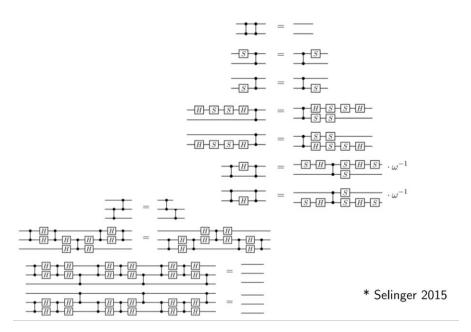
- Why use ZX-Calculus for this?
- Circuit simplifications also exist for logic gates:





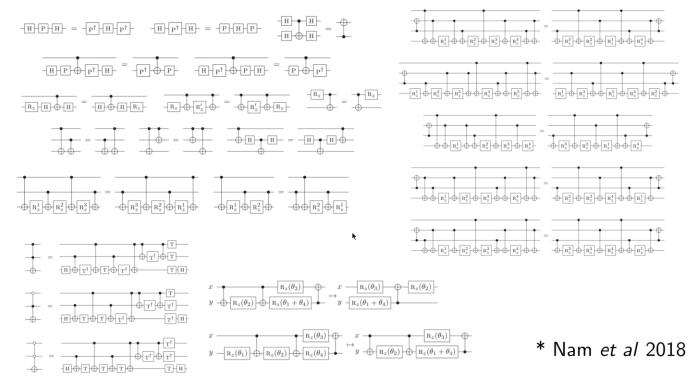
Unfortunately, there are more ...

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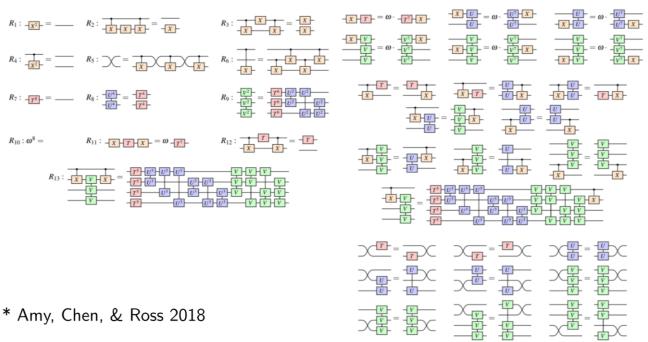


And more ...





And even more ...



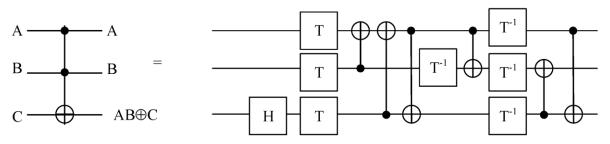


- Optimizing a circuit classically is unpractical
 - Finding an optimal simplification path is hard
 - Huge number of identities to consider
- ZX-Calculus solves this problem
 - It has a massively reduced set of simplification rules
 - Finding the optimal path is still hard, but it's manageable

T-Count Optimization



- Quantum computers are affected by noise
- Clifford+T Circuits can be made tolerant to noise (Error correcting codes)
 - Problem: Many new T-Gates need to be introduced
 - Difficult to simulate (Hardware Limits, high latency)
- ZX-Calculus can simplify such circuits

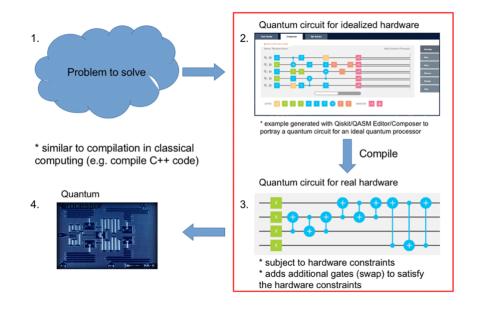


Decomposition of a Toffoli Gate: TCount = 7

Quantum Circuit Compilation



- Circuits use many abstract gates
- Problems of real quantum computers:
 - Limited set of gates
 - Limited connectivity between qubits
 - Noise
- Special circuit transformations
 - To swap qubits, so they can be entangled
 - Reduce the depth of circuits (noise issues)
 - Allow only some sets of gates
- ZX-Calculus can solve this
 - Can try to stick to those rules during the reconstruction phase

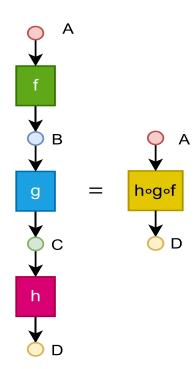


Mathematical Background: Category Theory



- Category C consists of objects and arrows (/morphisms)
 - − Objects: {*A*, *B*, *C*, *D*}
 - Morphisms: $f: A \rightarrow B$, $g: B \rightarrow C$, $h: C \rightarrow D$
- Every object *A* has an identity function
 - $-id_{A}:A\rightarrow A$
 - Represent *loops* in the diagram
- Naturally there exists an associative Composition (o)
 - Which is just the application of f and then g in a sequence
 - Example: $g \circ f : A \rightarrow C$
 - Composition with id does nothing

$$-id_B \circ f = f \circ id_A = f : A \to B$$



$$h \circ g \circ f : A \to D$$

Extension: Monoidal Category



Extend a Category C with:

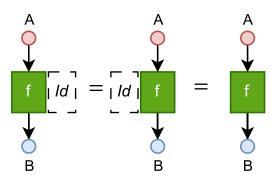
- An associative Bifunctor: ⊗: C × C → C
- A special object I ∈ obj(C) with
 - $-A \otimes I = A \otimes I = A$ for all objects A

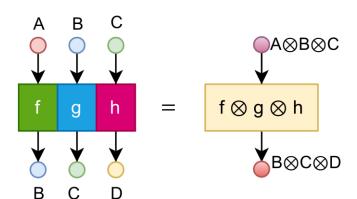
Example:

- For the morphisms: $f: A \rightarrow B$, $g: B \rightarrow C$, $h: C \rightarrow D$
- We can apply them in parallel

$$- f \otimes g \otimes h : A \otimes B \otimes C \rightarrow B \otimes C \otimes D$$

- So far: Very similar to regular circuit calculations
 - Matrix product for sequential gates
 - Tensor product for parallel gates

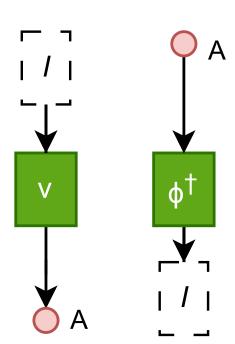




Special morphisms in Monoidal Categories



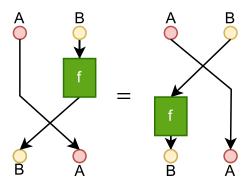
- Preparing States:
 - ν : I → A (Ket)
 - Creates State A out of nothing
- Erasing States:
 - $-\phi^{\dagger}$: $A \rightarrow I$ (Bra)
 - Deletes state A

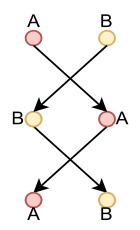


Extension: Symmetric Monoidal Category



- Extend a Monoidal Category C with:
 - Special tensor product: Swap isomorphism
 - $\ \sigma_{A,B}:A\otimes B\to B\otimes A$
 - For all $A, B \in obj(C)$
- Some other rules must hold:
 - "Push through" rule
 - "Double Swap = Identity" rule





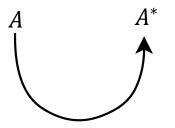
Extension: Compact Monoidal Category

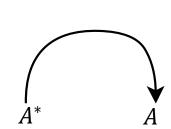


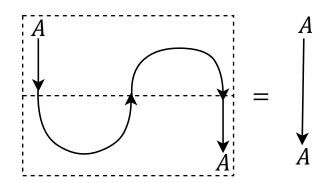
- If a monoidal category \mathcal{C} has:
 - A dual object A^* for every object $A \in obj(C)$
 - Special morphisms:
 - Unit: $\eta_A: I \to A^* \otimes A$ - Counit: $\epsilon_A: A \otimes A^* \to I$
- The combining rule must hold:
 - Meaning: $(\epsilon_A \otimes id_A) \circ (id_A \otimes \eta_A) = id_A$ for all $A \in obj(\mathcal{C})$
 - "Push through" rule also holds
- Why do all this mathematical mess?
 - It can just be seen graphically!
 - Just follow the lines
 - "Only Topology Matters"



$$\eta_A:I\to A^*\otimes A$$







Example Network

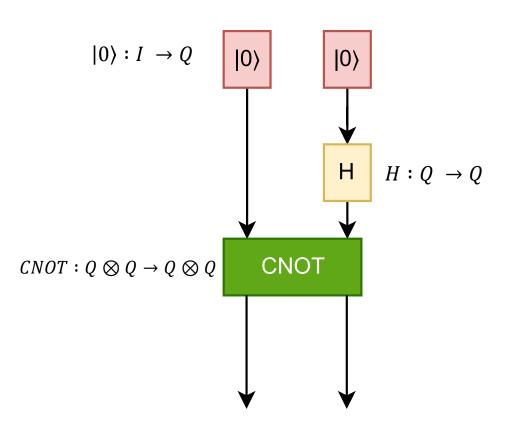


Concrete Category: FDHilb

- Objects: Hilbert Spaces / (Vector Spaces)
 - Concrete $I = \mathbb{C}$, $Q = \mathbb{C}^n$
- Morphisms: Linear Maps
 - $-m=\mathbb{C}^{m\times n}$
- Tensor Product: Kronecker Product
- Composition: Matrix Product

Skeleton of Entanglement Circuit

- 1. Create two |0> States
- 2. Apply Hadamard
- 3. Apply CNOT

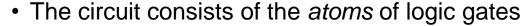


ZX-Notation

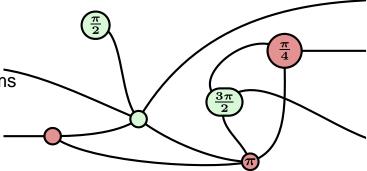


Main idea of ZX-Calculus

- Represent quantum circuits visually as a network of morphisms
- Apply simplifications on the network
- "Only topology Matters"
 - If it looks like the same graph, it's the same thing
 - Guaranteed by the rules of the underlying Category



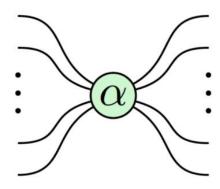
- We represent these atoms using spiders
- Spiders represent the morphisms from before

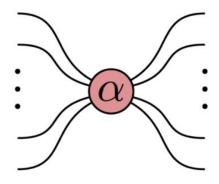


<u>Spiders</u>



- Spiders are the nodes in the graph
 - Arbitrary number of inputs/outputs
 - Represent linear maps
- Spider variations:
 - Green
 - Defined using eigenbasis of Z matrix
 - Red
 - Defined using eigenbasis of X matrix
 - Can have a phase angle α





Spiders as linear maps



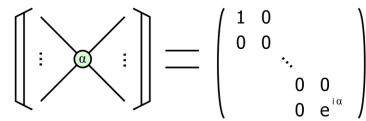
Each spider is a linear map

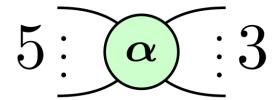
$$- GreenSpider(n,m)_{\alpha} = \underbrace{|0 \dots 0\rangle\langle 0 \dots 0|}_{m} + e^{i\alpha}\underbrace{|1 \dots 1\rangle\langle 1 \dots 1|}_{m}$$

$$- RedSpider(n,m)_{\alpha} = \underbrace{(+\cdots+)}_{m}\underbrace{(+\cdots+)}_{n} + e^{i\alpha}\underbrace{(-\cdots-)}_{m}\underbrace{(-\cdots-)}_{n}$$



- GreenSpider(5,3)_{α} represents a $2^3 \times 2^5 = 8 \times 32$ matrix
 - Not unitary
 - Not even square
- Spiders extend circuits into non-dimensional matrices





Spiders for Basis States



- Spiders can represent States and Gates
 - Global scalars are omitted

• X-Basis:
$$GreenSpider(n,m)_{\alpha} = \underbrace{|0\dots0\rangle\langle 0\dots0|}_{m} + e^{i\alpha}\underbrace{|1\dots1\rangle\langle 1\dots1|}_{m}$$

- GreenSpider
$$(0,1)_0 = |0\rangle \cdot 1 + e^{i\cdot 0}|1\rangle \cdot 1 = \begin{bmatrix} 1\\1 \end{bmatrix} \propto |+\rangle$$

- GreenSpider
$$(0,1)_{\pi} = |0\rangle \cdot 1 + e^{i \cdot \pi} |1\rangle \cdot 1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \propto |-\rangle$$

• **Z-Basis:**
$$RedSpider(n,m)_{\alpha} = \underbrace{\lfloor + \cdots + \rangle \langle + \cdots + \rfloor}_{m} + e^{i\alpha} \underbrace{\lfloor - \cdots - \rangle \langle - \cdots - \rfloor}_{m}$$

-
$$RedSpider(0,1)_0 = |+\rangle \cdot 1 + e^{i \cdot 0}|-\rangle \cdot 1 = \begin{bmatrix} 2 \\ 0 \end{bmatrix} \propto |0\rangle$$

-
$$RedSpider(0,1)_{\pi} = |+\rangle \cdot 1 + e^{i \cdot \pi}|-\rangle \cdot 1 = \begin{bmatrix} 0 \\ 2 \end{bmatrix} \propto |1\rangle$$

$$\bigcirc - = |+\rangle$$

$$\pi$$
 = $|-\rangle$

$$\bigcirc - = |0\rangle$$

$$\pi$$
 = $|1\rangle$

Spiders for Pauli Matrices



• Pauli-Z:
$$GreenSpider(n,m)_{\alpha} = \underbrace{|0\dots 0\rangle\langle 0\dots 0|}_{m} + e^{i\alpha}\underbrace{|1\dots 1\rangle\langle 1\dots 1|}_{m}$$

$$-(\pi)$$
 = 2

- GreenSpider
$$(1,1)_{\pi} = |0\rangle\langle 0| + e^{i\cdot\pi}|1\rangle\langle 1| = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = Z$$

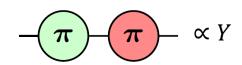
• Pauli-X:
$$RedSpider(n,m)_{\alpha} = \underbrace{\lfloor + \cdots + \rfloor}_{m} \underbrace{\langle + \cdots + \rfloor}_{n} + e^{i\alpha} \underbrace{\lfloor - \cdots - \rfloor}_{m} \underbrace{\langle - \cdots - \rfloor}_{n}$$

$$-(\pi)$$
 = X

-
$$RedSpider(1,1)_{\pi} = |+\rangle\langle+| + e^{i\cdot\pi}|-\rangle\langle-| = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = X$$

Pauli-Y: (Use commutation rules of Pauli Gates)

$$- RedSpider(1,1)_{\pi} \circ GreenSpider(1,1)_{\pi} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \circ \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \propto Y$$



Spider for Identity Matrix



- Every spider of arity 2 and phase angle $\alpha = 0$ is an identity matrix
 - If spider has no angle, it implicitly means $\alpha = 0$

- GreenSpider
$$(1,1)_0 = |0\rangle\langle 0| + e^{i\cdot 0}|1\rangle\langle 1| = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = id_2$$

$$- RedSpider(1,1)_0 = |+\rangle\langle +| + e^{i\cdot 0}| -\rangle\langle -| = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = id_2$$

- This is an important rewrite rule!
 - Identity spiders can be removed from the diagram

Spider for Bell State



Spiders can generate entangled States

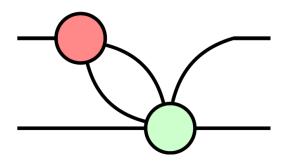
$$- GreenSpider(0,2)_0 = |00\rangle \cdot 1 + e^{i \cdot 0}|11\rangle \cdot 1 = \begin{bmatrix} 1\\0\\0\\1 \end{bmatrix} \propto |\Phi^+\rangle$$

- Using the identity rule from before we get a CAP
 - |Φ⁺⟩ represent the Unit-Morphism from the compact monoidal category

Combining Spiders



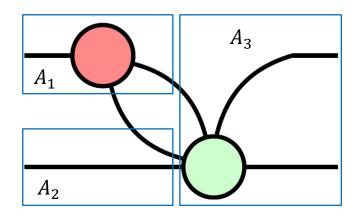
- Bigger Graphs can be constructed by connecting spiders
 - Every output of a spider gets connected to the input of another spider
 - Again: Only Topology matters
- The resulting graph can represent a quantum circuit
 - But not every graph is a valid circuit



Calculating a Graph



- To calculate the matrix representation
 - Divide the graph into regions
 - Each region must contain exactly one spider
- Simplification works just like normal circuits
 - "parallel" parts are combined using the tensor product
 - "sequential" parts are combined using the matrix product
- The resulting matrix represents the circuit
 - It is not necessary square / unitary



Example: CNOT

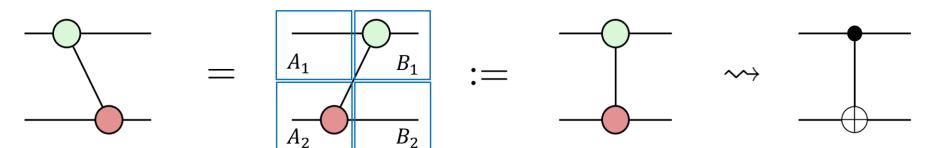


1. Evaluate parallel Sections

- $-A = A_1 \otimes A_2 = id_2 \otimes RedSpider(1,2)$
- $-B = B_1 \otimes B_2 = GreenSpider(2,1) \otimes id_2$

2. Combine sequential Regions

- $CNOT = B \circ A$

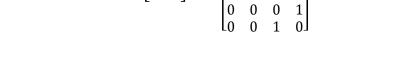


Example: CNOT Parallel Sections

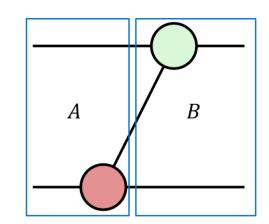


• $A = id_2 \otimes RedSpider(1,2) = id_2 \otimes (|+\rangle\langle ++|+|-\rangle\langle --|)$

$$-A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$



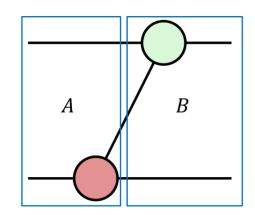
•
$$B = GreenSpider(2,1) \otimes id_2 = (|00\rangle\langle 0| + |11\rangle\langle 1|) \otimes id_2$$

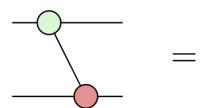


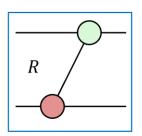
Example: CNOT Sequential Sections

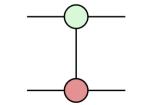


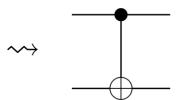
•
$$R = B \circ A$$











Where to draw the Regions?



- There may exist multiple ways of drawing the regions
 - Obvious, as you are allowed to move components around
 - "Only topology matters"
- This leads to different matrices in the calculation process
 - But the final matrices are always equivalent
 - (neglecting the global scalar factor)
- But why do it this way?
 - It is just as bad as the classical matrix approach

(a) Equivalent layouts of a CZ gate

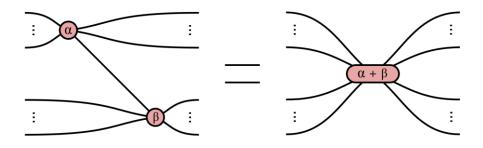
(b) Sign introduced by the transposition of a Y gate

$$= \overline{\underline{Y}} = (-1)$$

Simplification Rules



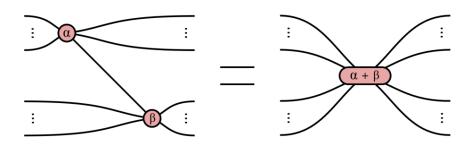
- We don't want to calculate the graph using its matrix form
- There exist many rules to simplify ZX-Graphs
 - But far fewer rules as for classical circuits
- We can apply the rules anywhere in the graph if:
 - The pattern for the substitution matches
 - The order of the input/output wires of regions is unchanged
 - All rule still holds if the spiders flip colors

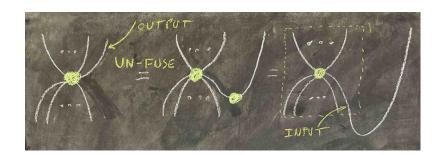


Spider Fusion



- Idea: Two spiders of the same color fuse together
 - Phase angles add up
 - Can simplify the graph a lot
- This rule allows to freely change input and outputs!
 - Only topology matters

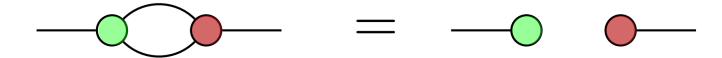




Hopf Rule



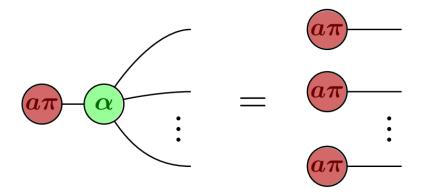
• Idea: 2 lines connecting 2 different colored spiders, can be deleted



Basis-State Copy Rules



- Idea: "Green copies Red", "Red copies Green"
 - Only works for computational basis states
 - $|0\rangle, |1\rangle/|+\rangle, |-\rangle$ depending on colors

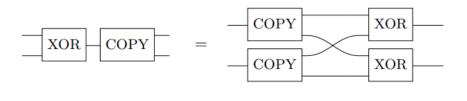


Bi-Algebra Rule



- Analog to digital logic
 - Create XOR using spider fusion
 - Use Copy-Rule from before



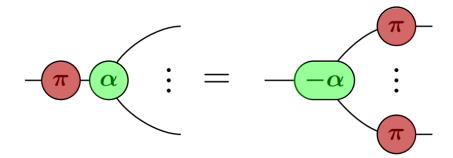




π -Commutation



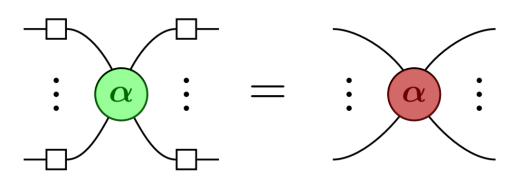
- Idea: A spider with angle π copy through a spider of opposite color
 - The phase of the other spider gets flipped



Color Change Rule



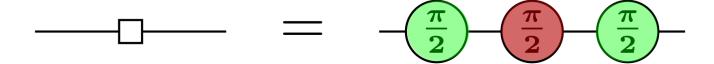
- Idea: We can change the color of a single spider
 - But we need to add Hadamard gates to all its inputs / outputs to compensate
- Analog: A Hadamard Gate can push through a spider
 - By copying itself to every other output



Hadamard Gate



- Hadamard Gates can be constructed using euler angles
 - Set up Hadamard as sequence of rotations



Hadamard Gate Cancelation

Two Hadamard Gates should cancel!

Using a visual proof, we see that the rule holds

— H— Н—

ТИП

 $\frac{\pi}{2}$ $\frac{\pi}{2}$ $\frac{\pi}{2}$

 $\frac{\pi}{2}$ (Translate to ZX)

 $-\left(\frac{\pi}{2}\right)-\left(\frac{\pi}{2}\right)-\left(\pi\right)$

(Spider-Fusion)

- $-\frac{\pi}{2}$
- $\frac{\pi}{2}$ $\frac{\pi}{2}$ $\frac{\pi}{2}$
- (π -Commutation)

 $-\frac{3\pi}{2}$ 0 $\frac{7}{2}$

(Spider-Fusion)



(Identity-Removal)



(Spider-Fusion)



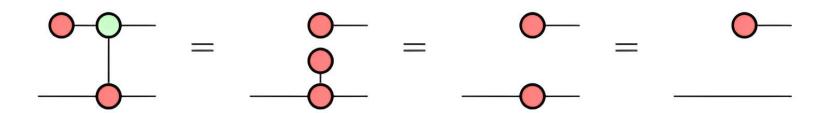
(Modulo)

(Identity-Removal)

Example CNOT Application: Control = $|0\rangle$



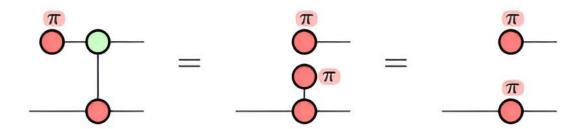
- As expected:
 - − |0⟩ Qubit passes through
 - Target qubit is untouched



Example CNOT Application: Control = |1>

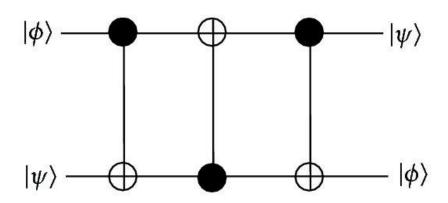


- As expected:
 - − |1⟩ Qubit passes through
 - Pauli X gate is applied to target qubit



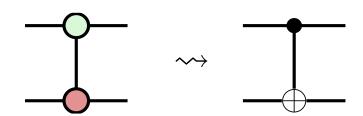


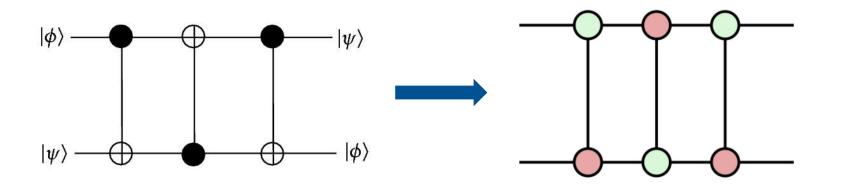
Circuit containing 3 alternating CNOTS





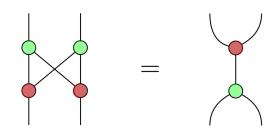
- Transform into ZX-Diagram
 - Remember CNOT Gate from earlier

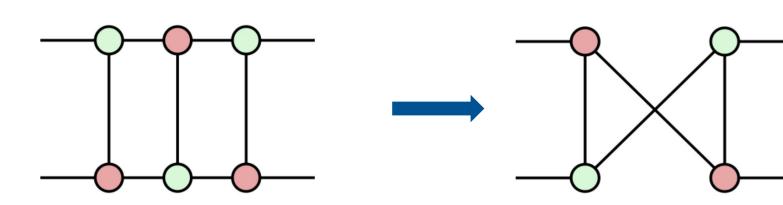




ТΙΠ

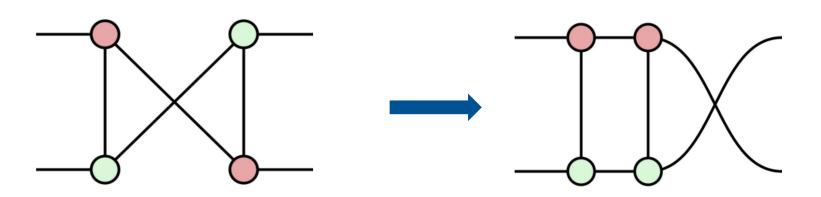
- Apply the bi-algebra rule
 - We need to morph the graph first!





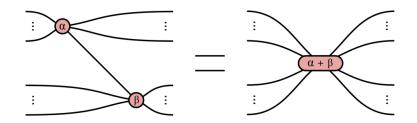


- Morph the ZX-Diagram
 - Allowed, since we are allowed to move stuff freely
 - Guaranteed by underlying category





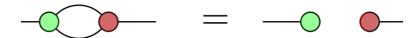
- Apply spider fusion rule
 - Attention, two wires remain between the first nodes!

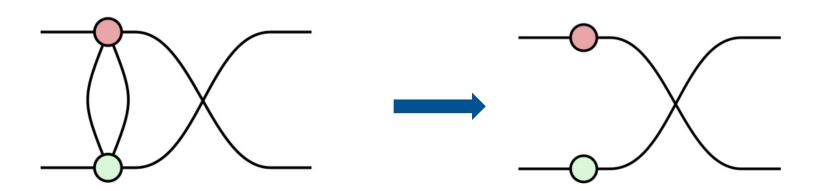






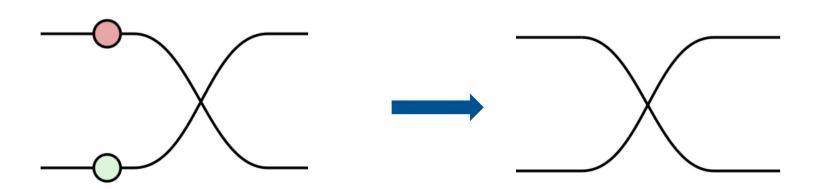
Apply the Hopf-Law





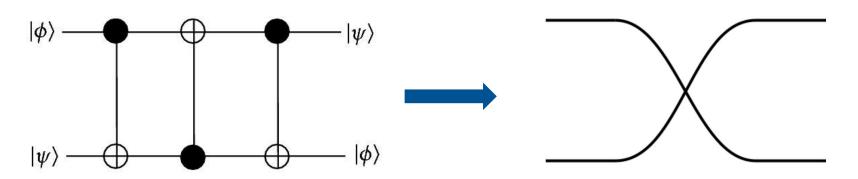


Identity Removal





- Complicated CNOT circuit is actually a swap operation
 - Since we are working at the atom-level many other circuits can be simplified like this
 - Extracting back quantum circuits is hard
 - But it's possible for simple circuits
 - (In general: Graph needs to have "gFlow")

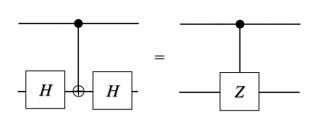


Translating Circuits



identity		$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
Pauli Z	(π)	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
Pauli X NOT gate		$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Pauli Y	i — (T)—	$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
Hadamard gate		$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1\\ 1 & -1 \end{pmatrix}$
S gate	$\left(\frac{\pi}{2}\right)$	$\begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$
V gate	$ \left(\frac{\pi}{2}\right)$ $-$	$\frac{1}{2} \begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}$
T gate	<u></u>	$\begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$

CNOT gate CX gate	$\sqrt{2}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
CZ gate	√2 -	$ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} $

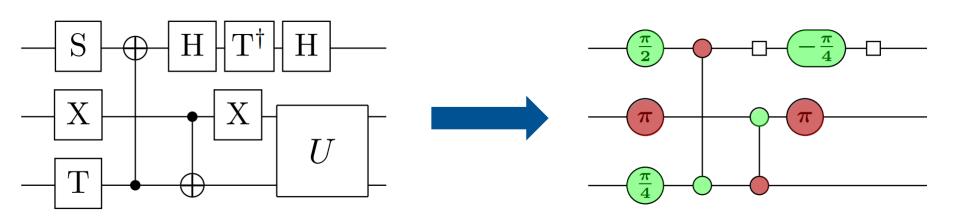


Challenge: Try to prove this identity!

From Quantum Circuits to ZX-Diagrams



- Example circuit:
 - Custom gates need to be handled separately
- Backwards direction also possible

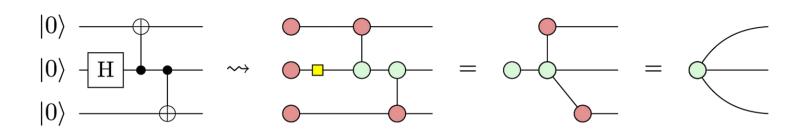


Example Circuit Simplification GHZ-State



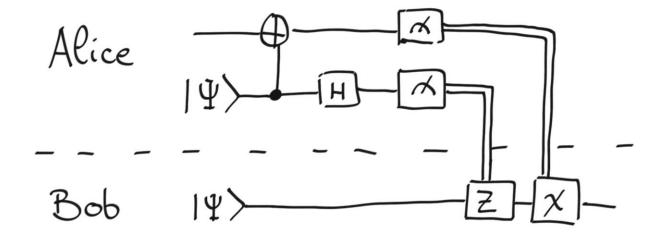
•
$$|GHZ\rangle = \frac{|000\rangle + |111\rangle}{\sqrt{2}}$$

- Calculating the circuit with ZX seems trivial compared to classical reasoning
 - $GreenSpider(0,3) = 1 \cdot |000\rangle + e^{i \cdot 0} \cdot 1 \cdot |111\rangle = |000\rangle + |111\rangle$



Quantum Teleportation

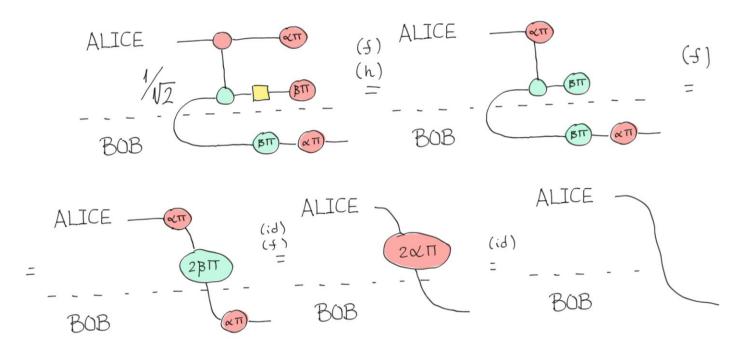




Quantum Teleportation



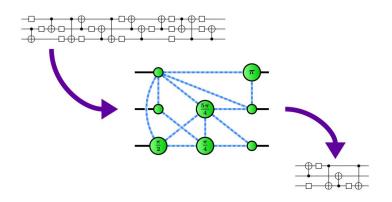
- Shared Bell State, is just a bent wire!
- Measurement is a parameterized spider

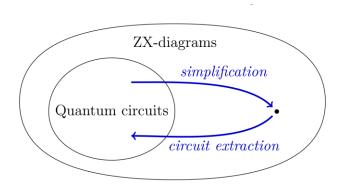


Completeness



- ZX Calculus is complete for Clifford+T gates
 - Any two ZX-Graphs for the same Quantum circuit can be transformed into each other
 - Since Clifford+T is approximately universal, ZX-Calculus is too
- This means that if a simpler circuit exists, it can be found using ZX-calculus
 - But the path between those transformations may traverse invalid quantum circuits





External Image Sources



- Quantum compilation [P.4]: https://quantum-journal.org/papers/q-2020-06-04-279/
- Circuit optimization [P.5]: https://quantum-journal.org/papers/q-2020-06-04-279/
- Circuit Identities: [P.6 P9]: https://arxiv.org/pdf/1310.6813.pdf
- Spiders as Matrix [P.20]: https://zxcalculus.com/tutorial
- CNOT ZX-Graph [P.27]: https://commons.wikimedia.org/wiki/File:ZX-calculus_cNOT-example.svg
- Example Circuit Identities [P.30]: https://www.arxiv-vanity.com/papers/2303.08829/
- Spider Fusion [P.32]: https://www.cs.ox.ac.uk/people/bob.coecke/ZX-lectures JPG.pdf
- CNOT Application [P.40 P.41]: https://quantumcomputing.stackexchange.com/questions/10235/explain-the-representation-of-the-cnot-gate-in-zx-calculus
- CNOT Simplification [P.43 P.48]: https://zxcalculus.com/
- Translating from Gates to ZX [P.50], Example Circuit [P.51]: https://arxiv.org/pdf/2012.13966.pdf
- GHZ State Simplification [P.52]: https://medium.com/quantinuum/how-zx-calculus-reveals-the-logic-and-processes-of-quantum-mechanics-to-everyone-944fc3bbbb2c
- Teleportation, Toffoli Gate Examples [P.53 P.56]: https://pennylane.ai/qml/demos/tutorial_zx_calculus
- Completeness [P.57]: https://arxiv.org/pdf/1902.03178.pdf