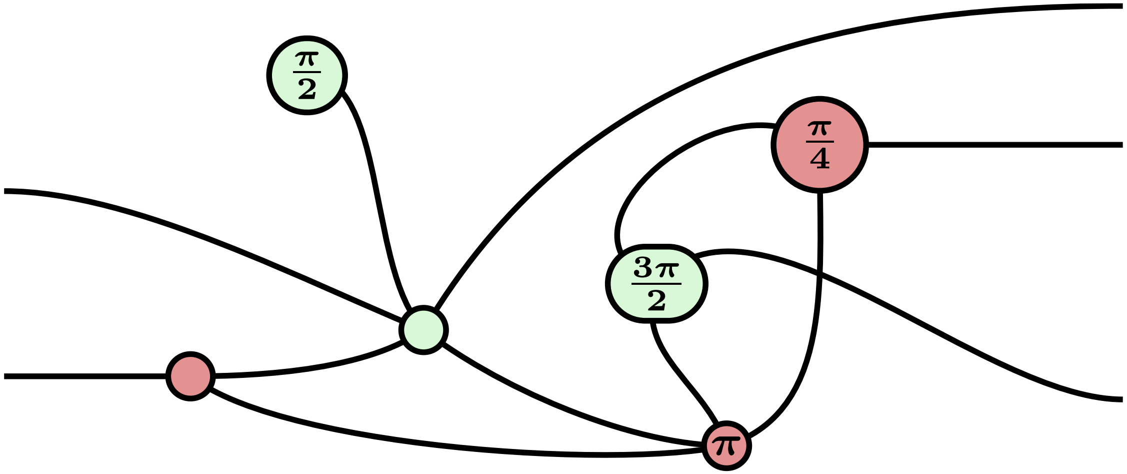
ZX-Calculus



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What is ZX-Calculus?

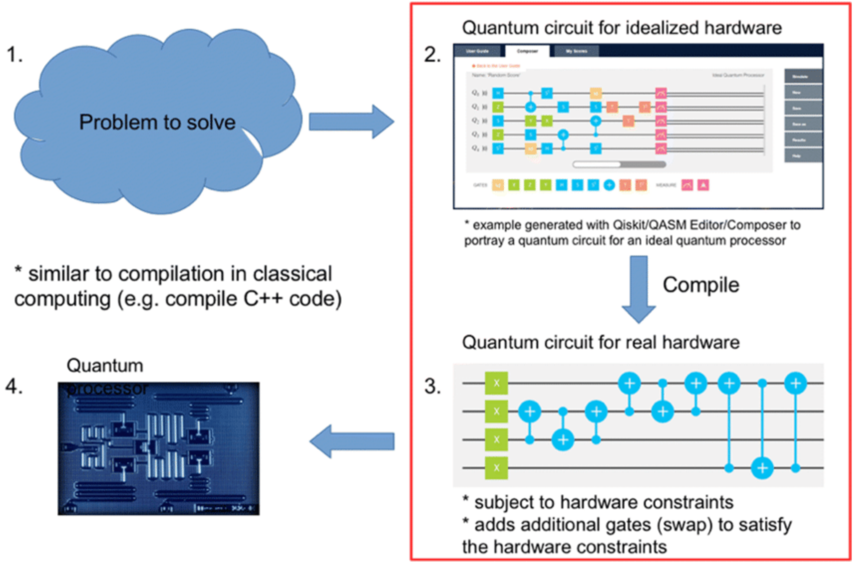
- A graphical language extending circuit diagrams
  - Allows breaking up logic gates into smaller *atoms*
  - The resulting graph is a *low-level* representation of the circuit
- Using transformations on those atoms we can visually deduce
  - Properties of circuits
  - Entangled states
  - How quantum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

Applications

- Quantum circuit optimization
  - Reduce 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

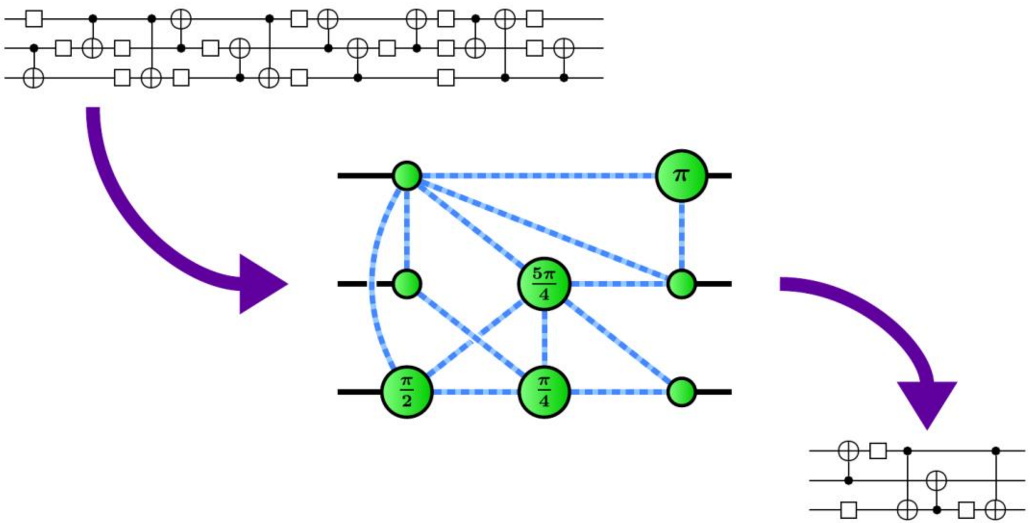
Quantum Circuit optimization

- 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 depth of circuit (noise issues)
  - Allow only some set of gates
- ZX-Calculus can solve this
  - Can try to stick to those rules during the reconstruction phase



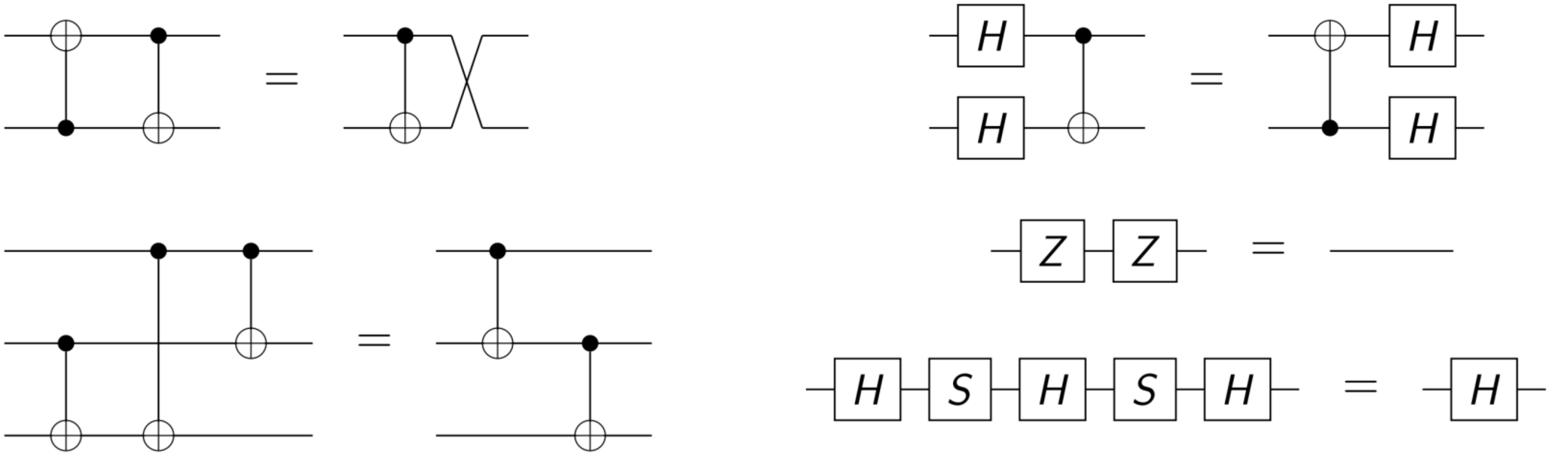
Quantum Circuit optimization

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



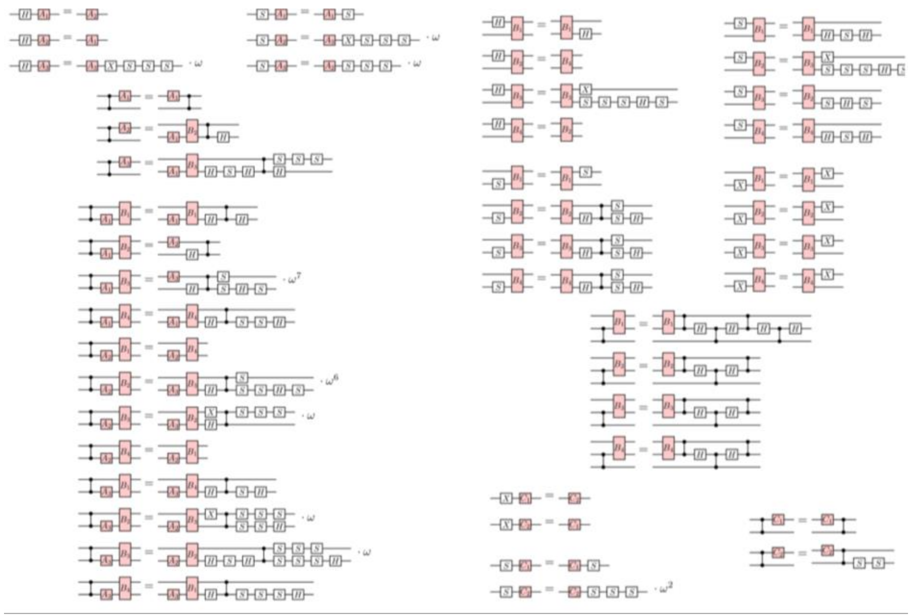
Classical optimization

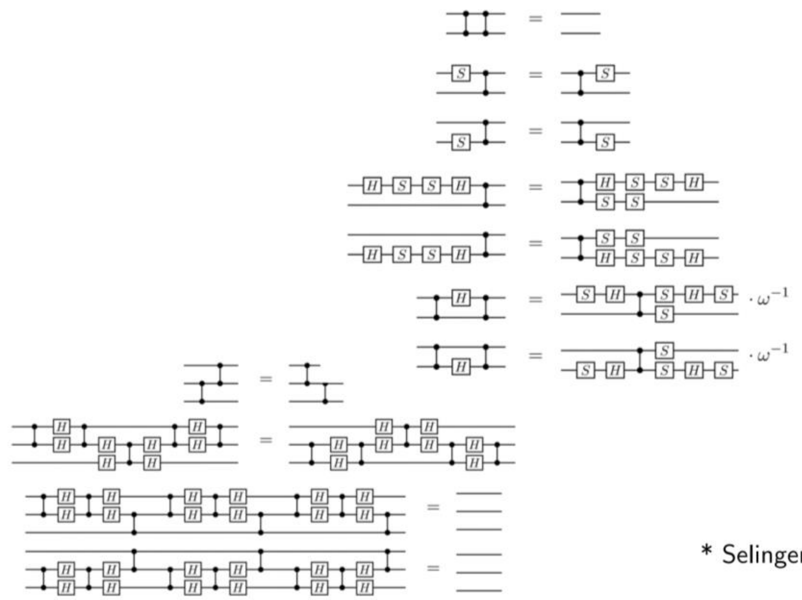
- Why use ZX-Calculus for this?
- Circuit simplifications also exist for logic gates:



Classical optimization

- Unfortunately, there are more …

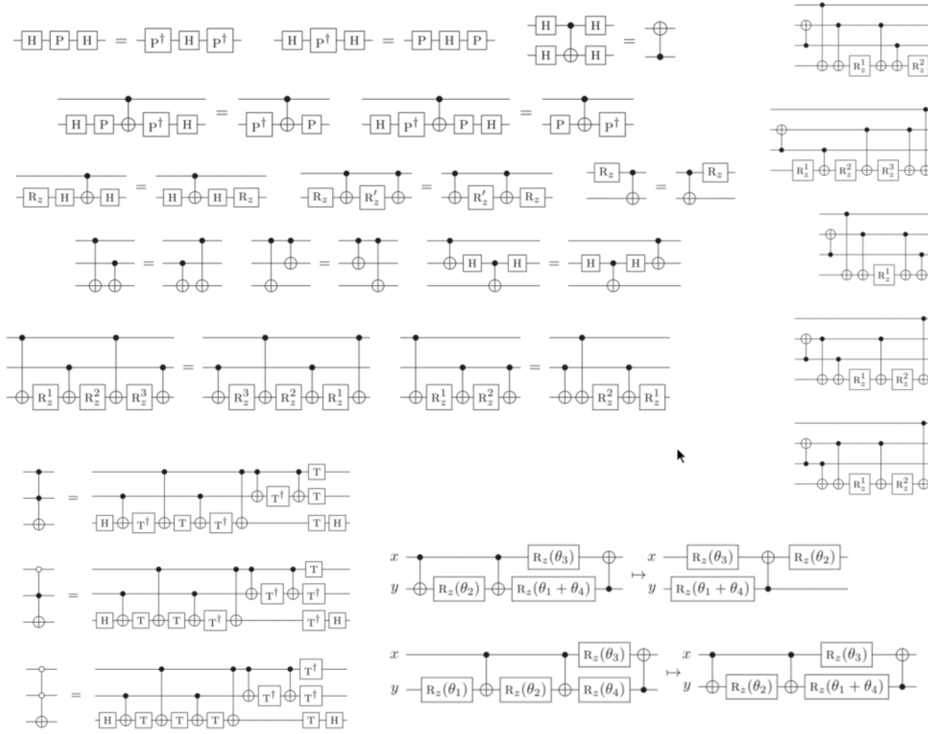


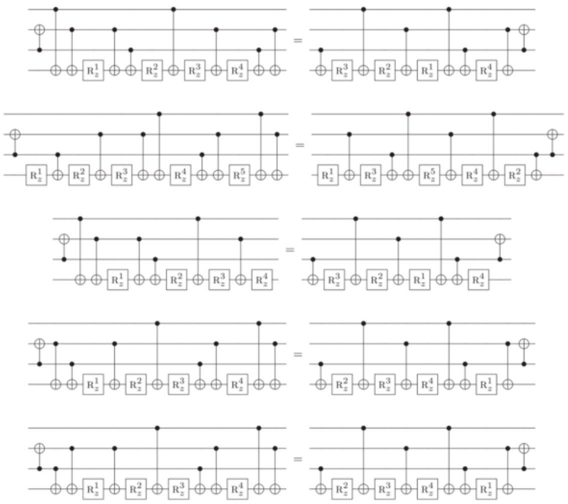


* Selinger 2015

Classical optimization

- And more …

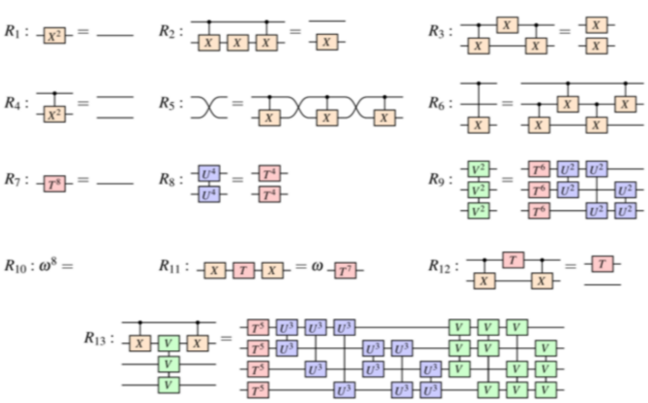


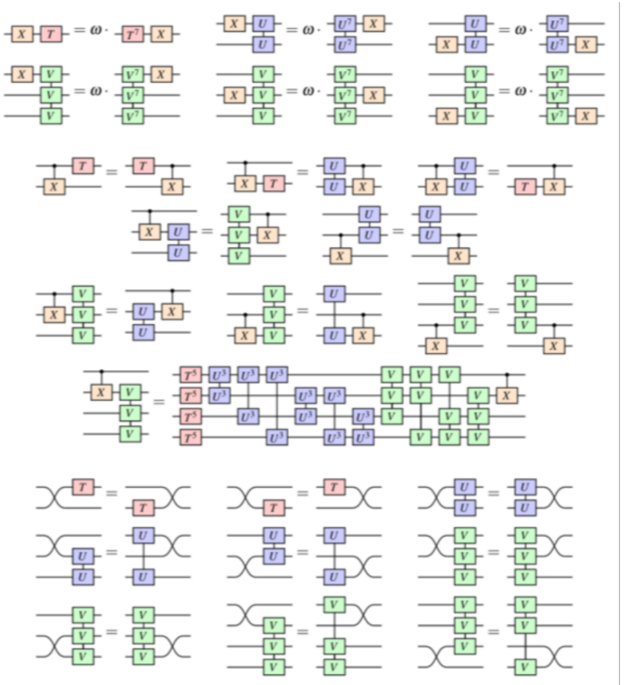


* Nam *et al* 2018

Classical optimization

- And even more …





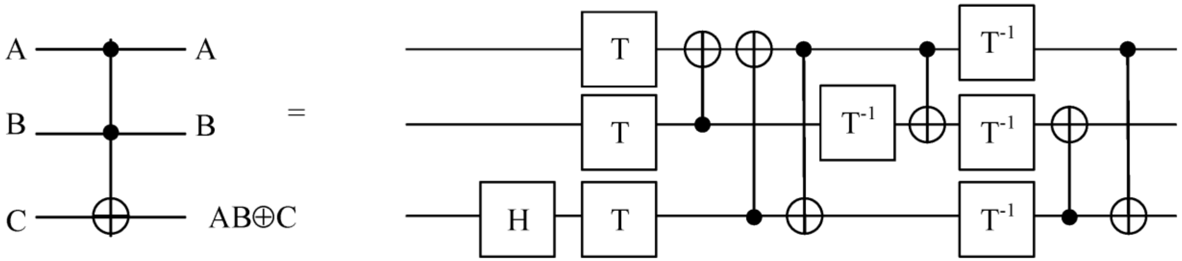
* Amy, Chen, & Ross 2018

Classical optimization

- 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 its manageable

T-Count Optimization

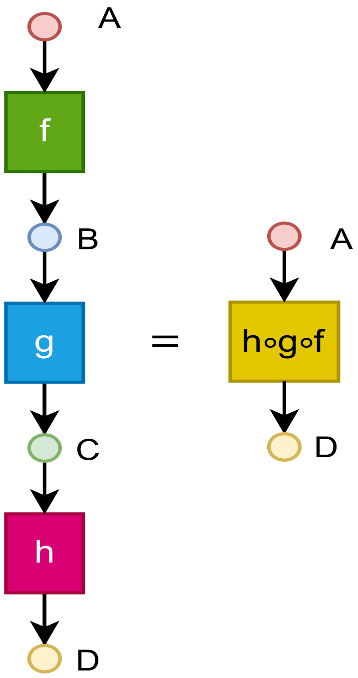
- Quantum computers are affected by noise
- Clifford+T Circuits can be made tolerant to noise
  - Problem: Many new T-Gates need to be introduced
  - Difficult to simulate (Hardware Limits, high latency)
- ZX-Calculus can simplify such circuits



Decomposition of a Toffoli Gate: TCount = 7

Mathematical Background: Category Theory

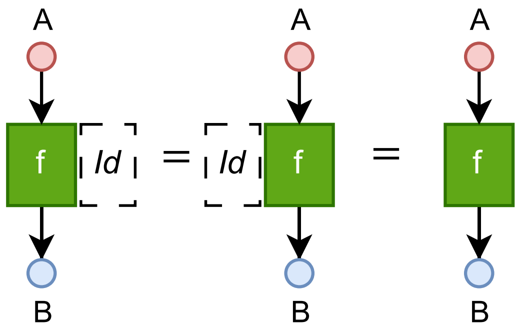
- Category $\mathcal{C}$ consists of **objects** and **arrows** (/morphisms)
  - Objects: $\{A, B, C, D\}$
  - Morphisms: $f : A \rightarrow B,\ g : B \rightarrow C,\ h : C \rightarrow D$
- Every object A has an identity function
  - $id_{\mathrm{A}} : A \rightarrow A$
  - Represent *loops* in the diagram
- Naturally there exists an associative Composition ($\circ$)
  - 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
    - $id_B \circ f = f \circ id_A = f \ : \ A \rightarrow B$



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

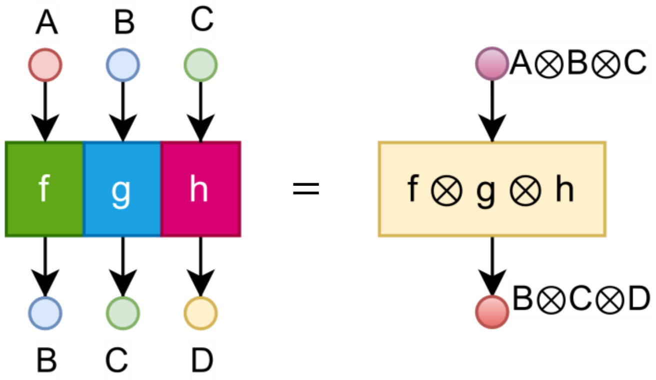
Extension: Monoidal Category

- Extend a Category $\mathcal{C}$ with:
  - An associative Bifunctor: $\otimes : \mathcal{C} \times \mathcal{C} \rightarrow \mathcal{C}$
  - A special object $I \in obj(\mathcal{C})$ with
    - $A \otimes I = A \otimes I = A$ for all objects A



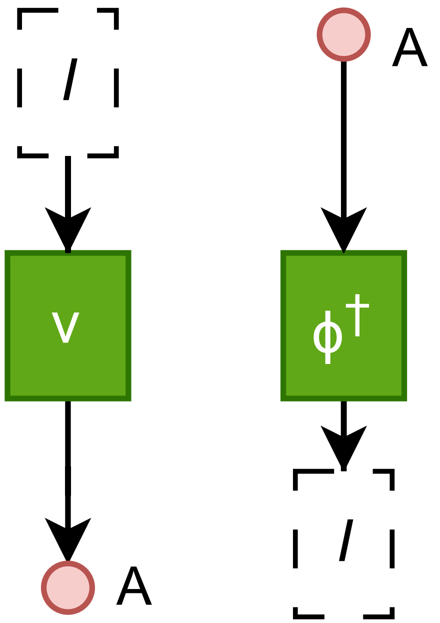
- Example:
  - For the morphisms: $f : A \rightarrow B,\ g : B \rightarrow C,\ h : C \rightarrow D$
  - We can *apply* them in *parallel*
    - $f \otimes g \otimes h : A \otimes B \otimes C \rightarrow B \otimes C \otimes D$

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



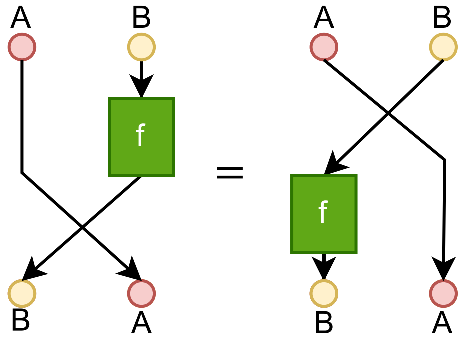
Special morphisms in Monoidal Categories

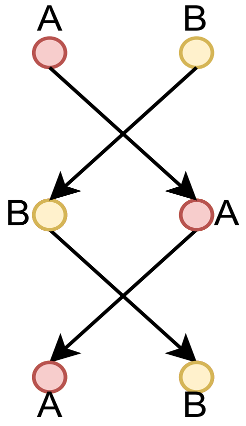
- Preparing States:
  - ν: $I \to A$ (Ket)
  - Creates State A out of nothing
- Erasing States:
  - $\phi^{\dagger}$: $A \to I$ (Bra)
  - Deletes state A



Extension: Symmetric Monoidal Category

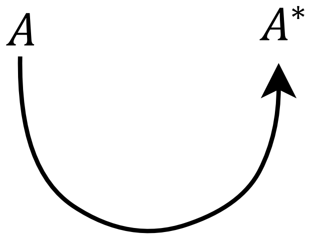
- Extend a Monoidal Category $\mathcal{C}$ with:
  - Special tensor product: Swap isomorphism
    - $\sigma_{A,B} : A \otimes B \to B \otimes A$
    - For all $A, B \in obj(\mathcal{C})$
- Some other rules must hold:
  - “Push through” rule
  - “Double Swap = Identity” rule

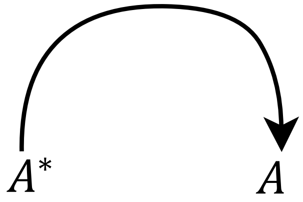




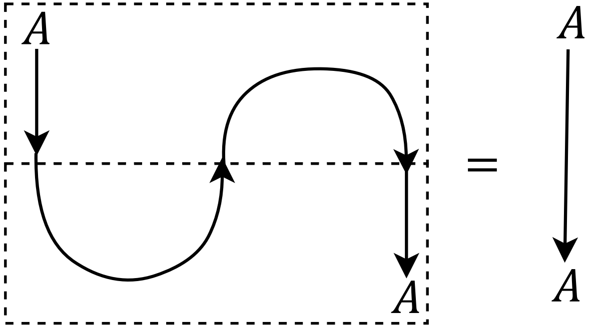
Extension: Compact Monoidal Category

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





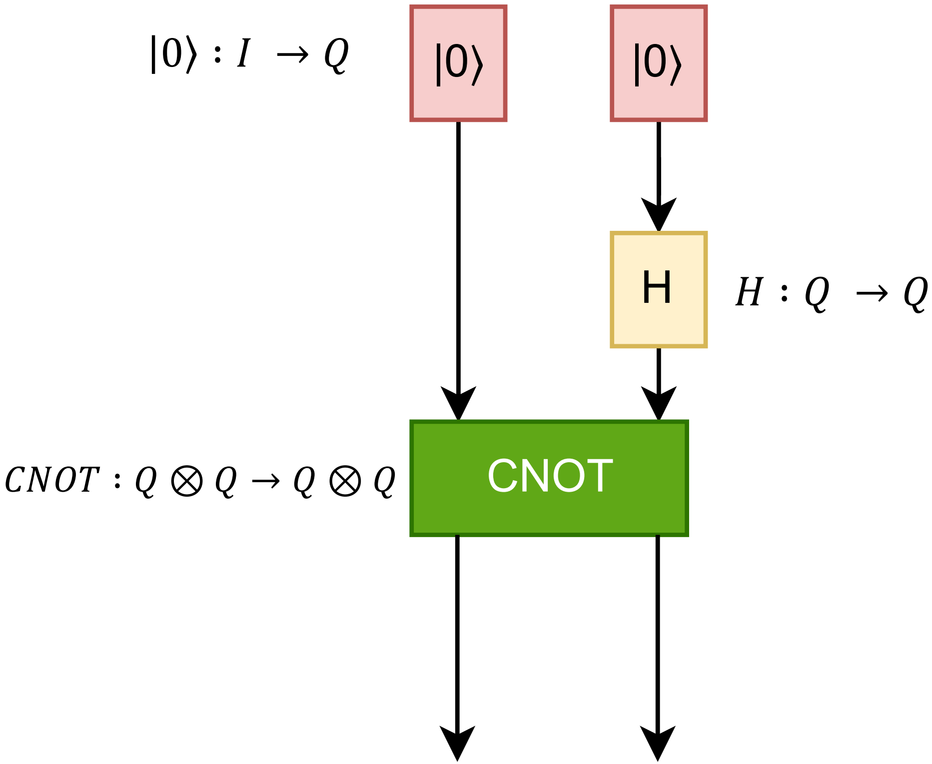
- If a monoidal category $\mathcal{C}$ has:
  - A dual object A^* for every object $A \in obj(\mathcal{C})$
  - Special morphisms:
    - *Unit:* $\eta_A : I \to A^* \otimes A$
    - *Counit:* $\epsilon_A : A \otimes A^* \to I$
- The combining rule must hold:
  - Meaning: $(\epsilon_A \otimes id_A) \circ (id_A \otimes \eta_A) = id_A$ 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”



Example Network

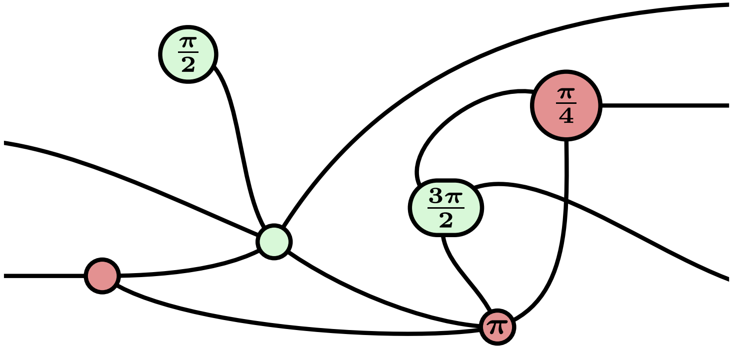
- Concrete Category: **FDHilb**
  - Objects: Hilbert Spaces / (Vector Spaces)
    - Concrete $I = \mathbb{C}, Q = \mathbb{C}^n$
  - Morphisms: Linear Maps
    - $m = \mathbb{C}^{m \times n}$
  - Tensor Product: Kronecker Product
  - Composition: Matrix Product

- Skeleton of Entanglement Circuit
  1. Create two $|0\rangle$ States
  2. Apply Hadamard
  3. Apply CNOT



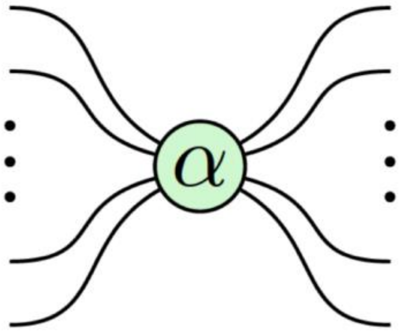
ZX-Notation

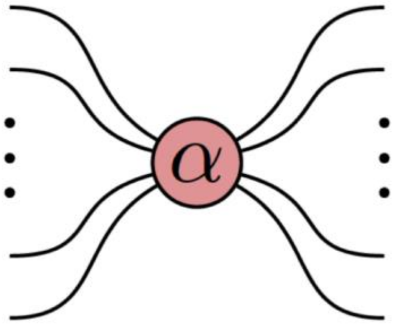
- Main idea of ZX-Calculus
  - Represent quantum circuit visually as network of morphisms
  - Apply simplifications on the network
  - “Only topology Matters”
    - If it looks like the same graph its the same thing
    - Guaranteed by the rules of the underlying Category
- The circuit consists of the *atoms* of logic gates
  - We represent this atoms using spiders
  - Spiders represent the morphisms from before



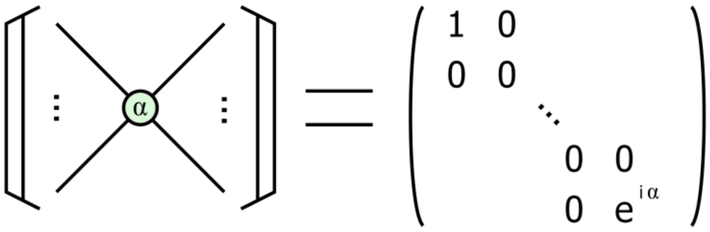
Spiders

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

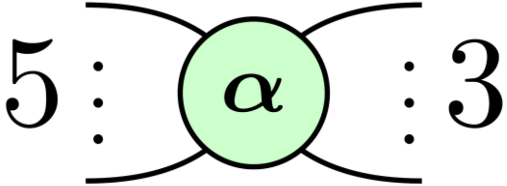




Spiders as linear maps



- Each spider is a linear map
  - $GreenSpider(n,m)_\alpha = |\underbrace{0 \dots 0}_{m}\rangle\langle\underbrace{0 \dots 0}_{n}| + e^{i\alpha}|\underbrace{1 \dots 1}_{m}\rangle\langle\underbrace{1 \dots 1}_{n}|$
  - $RedSpider(n,m)_\alpha = |\underbrace{+ \cdots +}_{m}\rangle\langle\underbrace{+ \cdots +}_{n}| + e^{i\alpha}|\underbrace{- \cdots -}_{m}\rangle\langle\underbrace{- \cdots -}_{n}|$
- Example Spider:
  - $GreenSpider(5,3)_\alpha$ represents a $2^3 \times 2^5 = 8 \times 32$ matrix
    - Not unitary
    - Not even square
  - Spiders extend classical gates into non-dimensional matrices

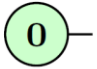


Spiders for Basis States

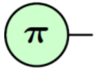
- Spiders can represent States **and** Gates
  - Global scalars are omitted

- **X-Basis:** $GreenSpider(n,m)_\alpha = |\underbrace{0 \ldots 0}_{m}\rangle\langle\underbrace{0 \ldots 0}_{n}| + e^{i\alpha}|\underbrace{1 \ldots 1}_{m}\rangle\langle\underbrace{1 \ldots 1}_{n}|$
  - $GreenSpider(0,1)_0 = |0\rangle \cdot 1 + e^{i \cdot 0}|1\rangle \cdot 1 = \begin{bmatrix}1\\1\end{bmatrix} \propto |+\rangle$
  - $GreenSpider(0,1)_\pi = |0\rangle \cdot 1 + e^{i \cdot \pi}|1\rangle \cdot 1 = \begin{bmatrix}1\\-1\end{bmatrix} \propto |-\rangle$

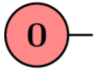
- **Z-Basis:** $RedSpider(n,m)_\alpha \quad = |\underbrace{+ \cdots +}_{m}\rangle\langle\underbrace{+ \cdots +}_{n}| + e^{i\alpha}|\underbrace{- \cdots -}_{m}\rangle\langle\underbrace{- \cdots -}_{n}|$
  - $RedSpider(0,1)_0 = |+\rangle \cdot 1 \ + e^{i \cdot 0}|-\rangle \cdot 1 = \begin{bmatrix}2\\0\end{bmatrix} \propto |0\rangle$
  - $RedSpider(0,1)_\pi = |+\rangle \cdot 1 \ + e^{i \cdot \pi}|-\rangle \cdot 1 = \begin{bmatrix}0\\2\end{bmatrix} \propto |1\rangle$



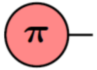
$= |+\rangle$



$= |-\rangle$



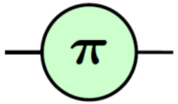
$= |0\rangle$



$= |1\rangle$

Spiders for Pauli Matrices

- **Pauli-Z:** $GreenSpider(n,m)_\alpha = |\underbrace{0 \dots 0}_{m}\rangle\langle\underbrace{0 \dots 0}_{n}| + e^{i\alpha}|\underbrace{1 \dots 1}_{m}\rangle\langle\underbrace{1 \dots 1}_{n}|$
  - $GreenSpider(1,1)_\pi = |0\rangle\langle 0| + e^{i\cdot\pi}|1\rangle\langle 1| = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = Z$

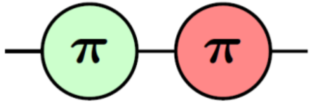


$= Z$

- **Pauli-X:** $RedSpider(n,m)_\alpha = |\underbrace{+ \cdots +}_{m}\rangle\langle\underbrace{+ \cdots +}_{n}| + e^{i\alpha}|\underbrace{- \cdots -}_{m}\rangle\langle\underbrace{- \cdots -}_{n}|$
  - $RedSpider(1,1)_\pi = |+\rangle\langle +| + e^{i\cdot\pi}|-\rangle\langle -| = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = X$

$= X$

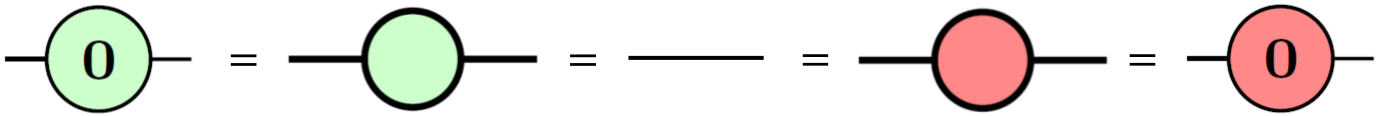
- **Pauli-Y:**
  - $RedSpider(1,1)_\pi \circ GreenSpider(1,1)_\pi = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \circ \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \propto Y$



$\propto Y$

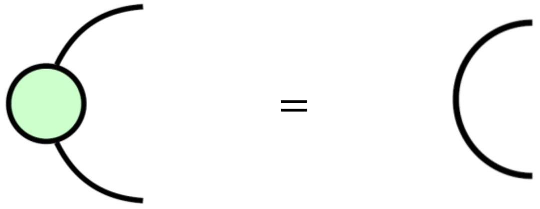
Spider for Identity Matrix

- 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 just be removed from the diagram



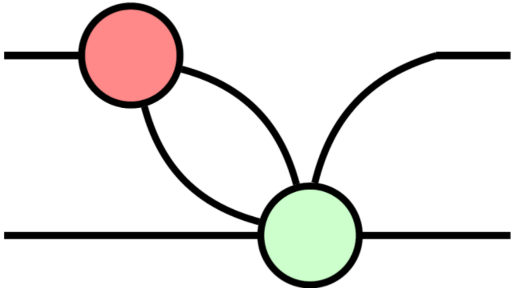
Spider for Bell State

- 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
  - $|\Phi^+\rangle$ represent the Unit-Morphism from the compact monoidal category



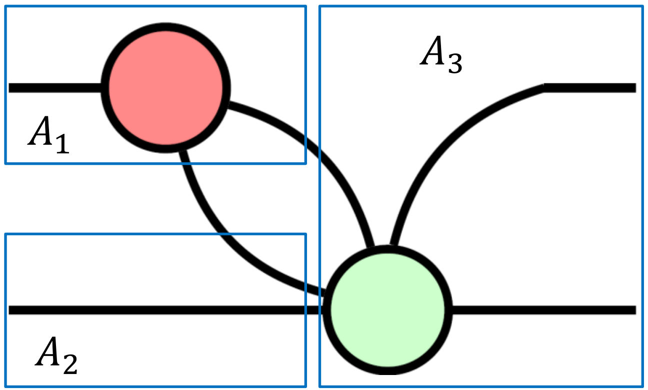
Combining Spiders

- 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

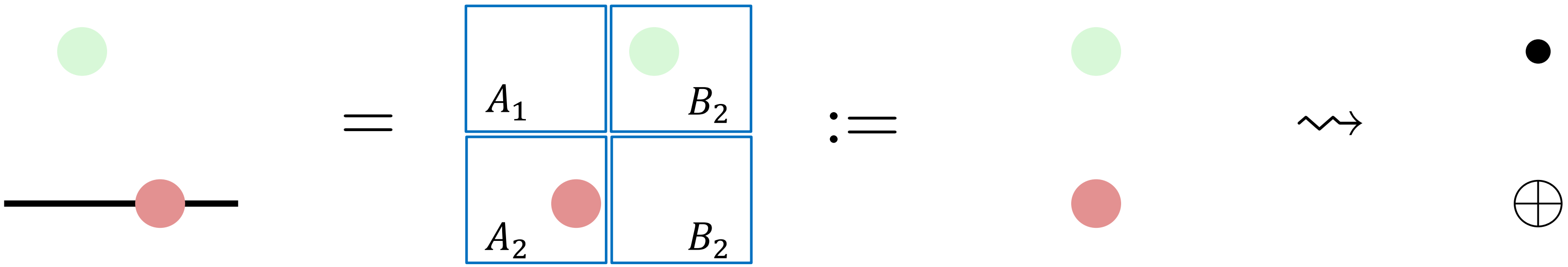
- To calculate the matrix representation
  - Divide the graph into regions
  - Each region must contain **exactly** one spider
- Simplification works just like normal circuits
  - “parallel” parts are combined using the tensor product
  - “sequential” parts are combined using the matrix product
- The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



Example: CNOT

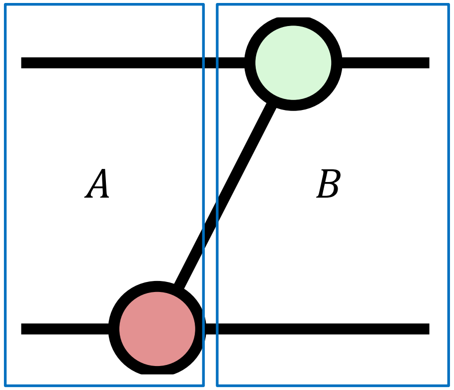
1. Evaluate parallel Sections
   - $A = A_1 \otimes A_2 = id_2 \otimes RedSpider(1, 2)$
   - $B = B_1 \otimes B_1 = GreenSpider(2,1) \otimes id_2$

2. Combine sequential Regions
   - $CNOT = B \circ A$

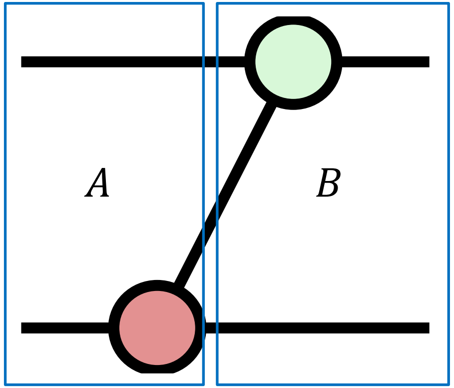


Example: CNOT Parallel Sections

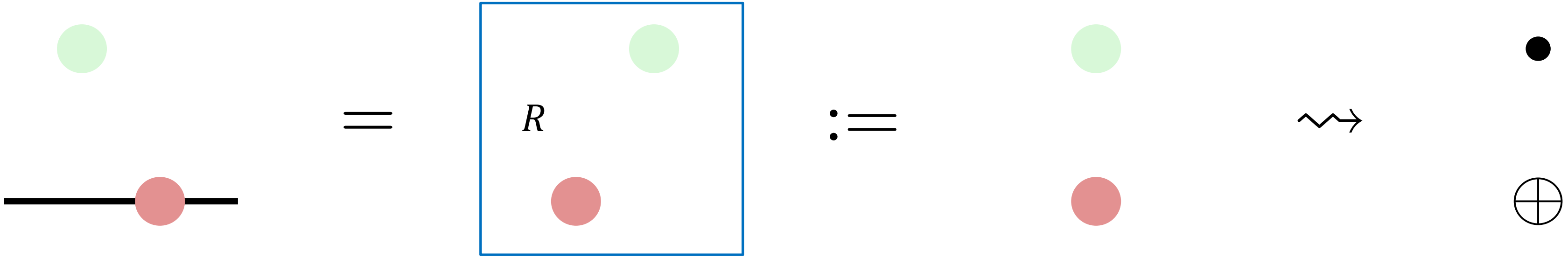
- $A = id_2 \otimes RedSpider(1,2) = \mathrm{id}_2 \otimes (\,|+\rangle\langle+\,+| + |-\rangle\langle-\,-|\,)$
  - $A = \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} \otimes \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0\\0 & 1\\0 & 1\\1 & 0\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 1 & 0 & 0\\1 & 0 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & 1\\0 & 0 & 0 & 1\\0 & 0 & 1 & 0\end{bmatrix}$
- $B = GreenSpider(2,1) \otimes id_2 = (\,|00\rangle\langle 0| + |11\rangle\langle 1|\,) \otimes id_2$
  - $B = \begin{bmatrix}1 & 0 & 0 & 0\\0 & 0 & 0 & 1\end{bmatrix} \otimes \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} = \begin{bmatrix}1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\0 & 1 & 0 & 0 & 0 & 0 & 0 & 0\\0 & 0 & 0 & 0 & 0 & 0 & 1 & 0\\0 & 0 & 0 & 0 & 0 & 0 & 0 & 1\end{bmatrix}$



Example: CNOT Sequential Sections

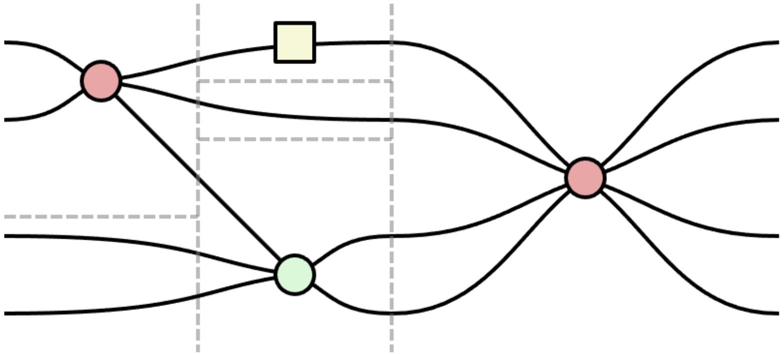


- $R = B \circ A$
  - $R = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \circ \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \propto CNOT$



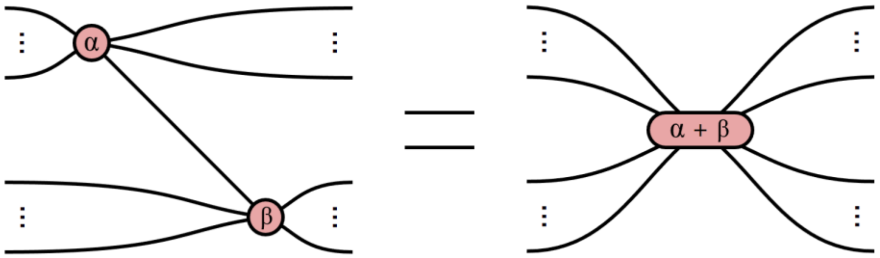
Where to draw the Regions?

- 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



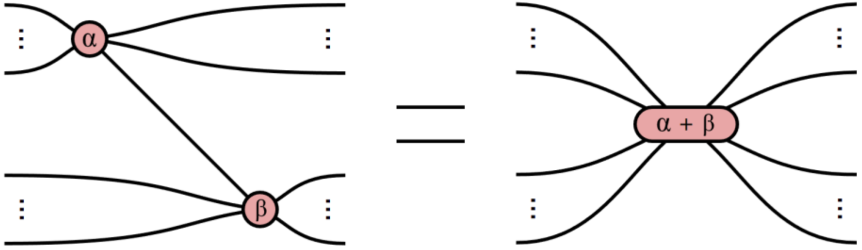
Simplification Rules

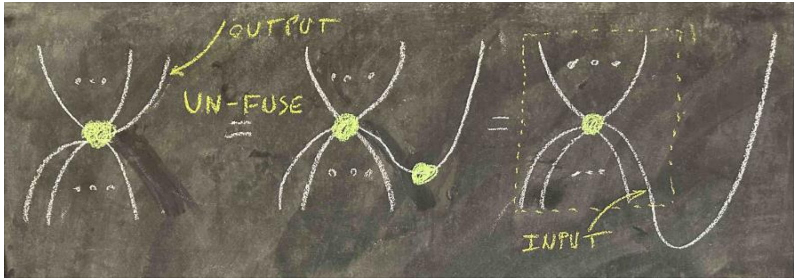
- We don’t want to calculate the graph using its matrix form
- There exist many rules to simplify ZX-Graphs
  - But far fewer rules as for classical circuits
- We can apply the rules anywhere in the graph if:
  - The pattern for the substitution matches
  - The order of the input / output wires of regions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



Spider Fusion

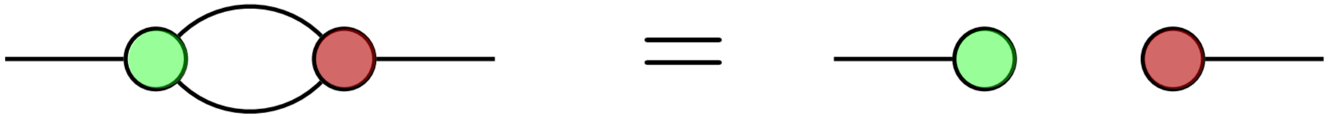
- Idea: Two spiders of the same color fuse together
  - Phase angles add up
  - Can simplify graph a lot
- This rule allows to freely change input and outputs!
  - Only topology matters





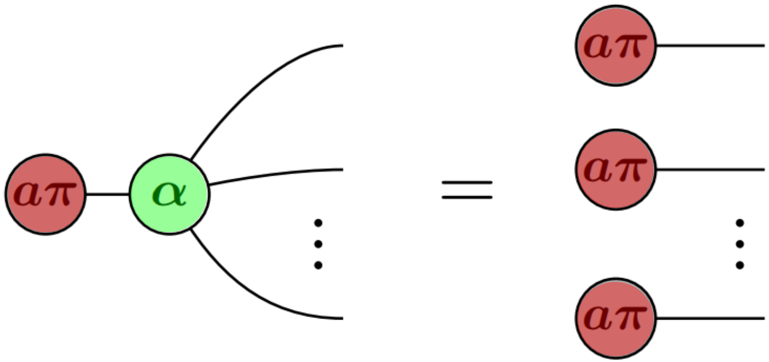
Hopf Rule

- Idea: If two spiders of different color are connected by 2 lines, both lines can be deleted



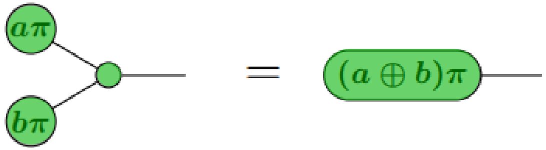
State Copy Rules

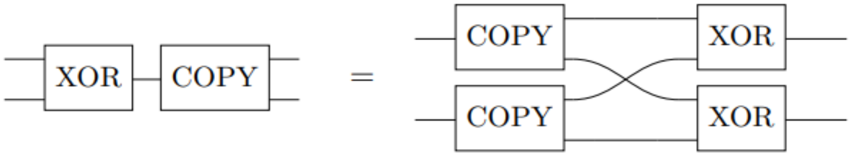
- Idea: “Green copies Red”, “Red copies Green”
  - Only works for computational basis states
    - $|0\rangle, |1\rangle$ / $|+\rangle, |-\rangle$ depending on colors

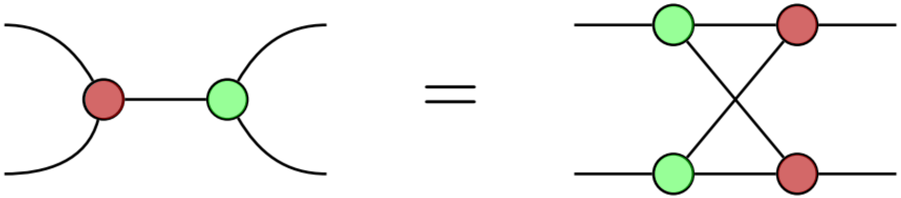


Bi-Algebra Rule

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

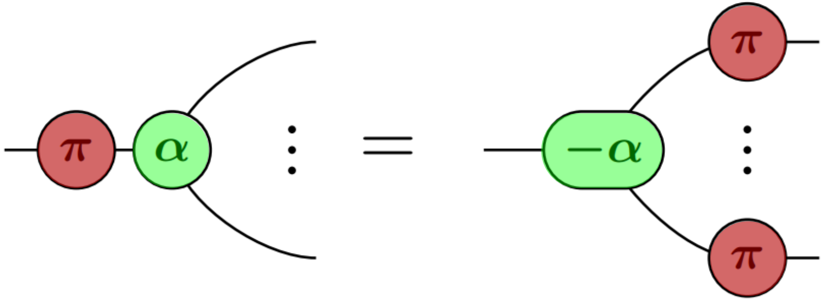






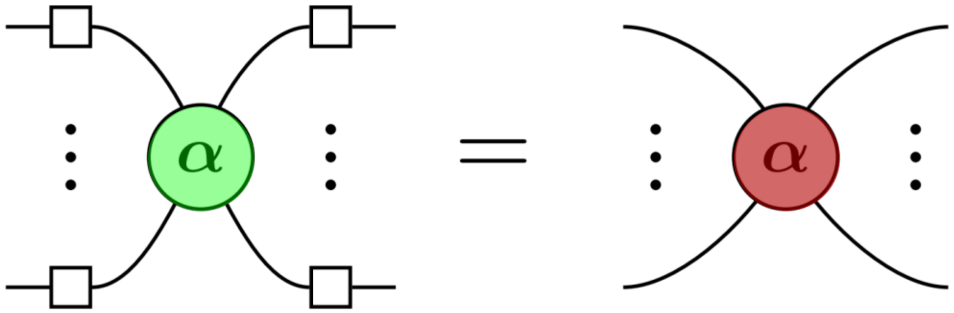
π-Commutation

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



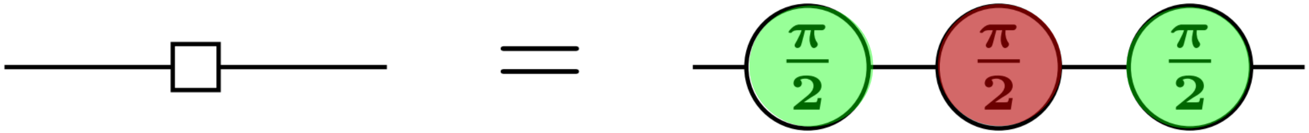
Color Change Rule

- 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



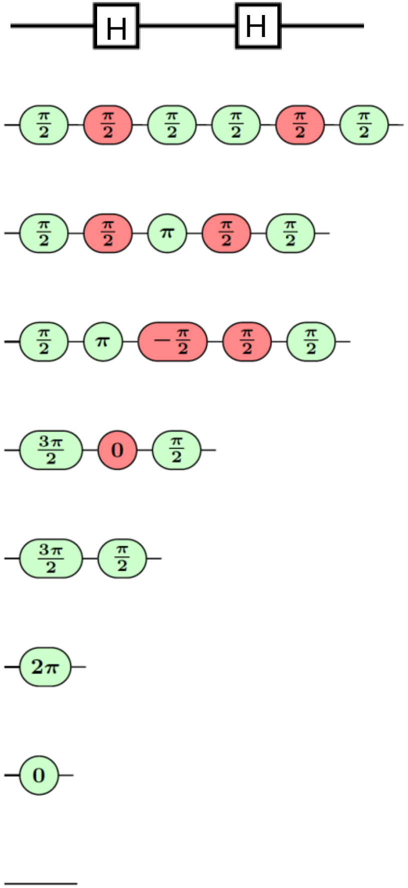
Hadamard Gate

- 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



(Translate to ZX)

(Spider-Fusion)

(π-Commutation)

(Spider-Fusion)

(Identity-Removal)

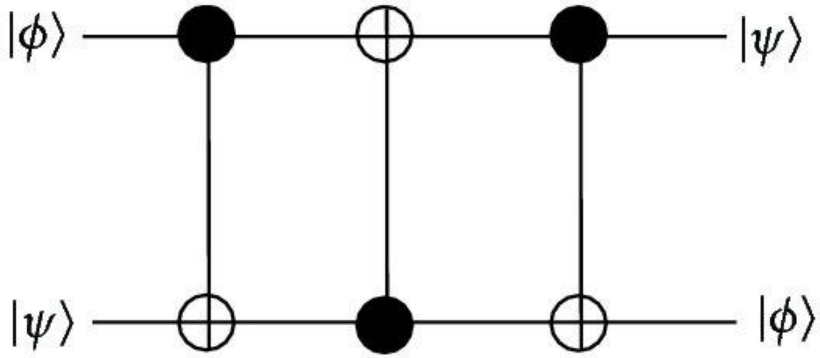
(Spider-Fusion)

(Modulo)

(Identity-Removal)

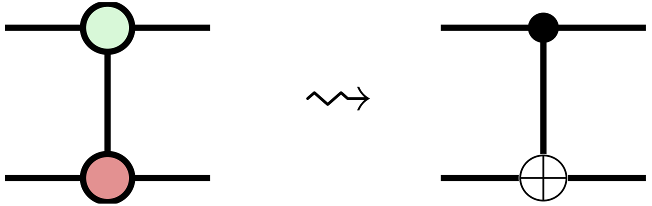
Simplification: Three CNOTs

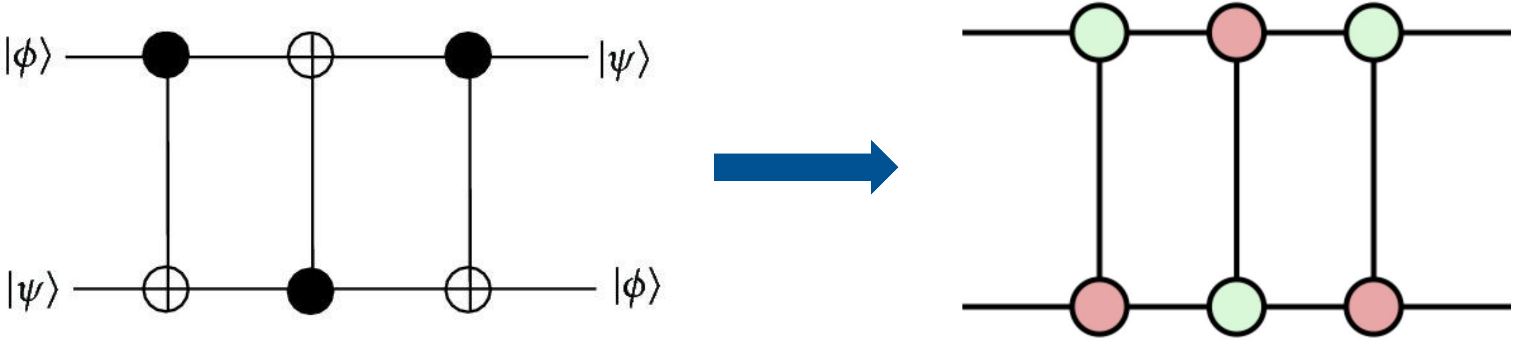
- Circuit containing 3 alternating CNOTS



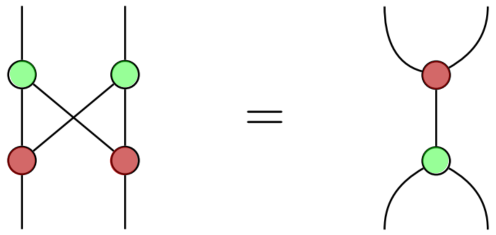
Simplification: Three CNOTs

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





Simplification: Three CNOTs

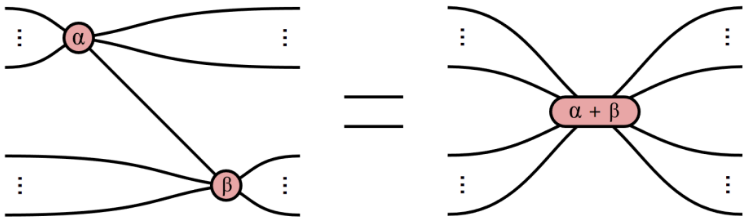


- Apply the bi-algebra rule
  - We need to morph the graph first!

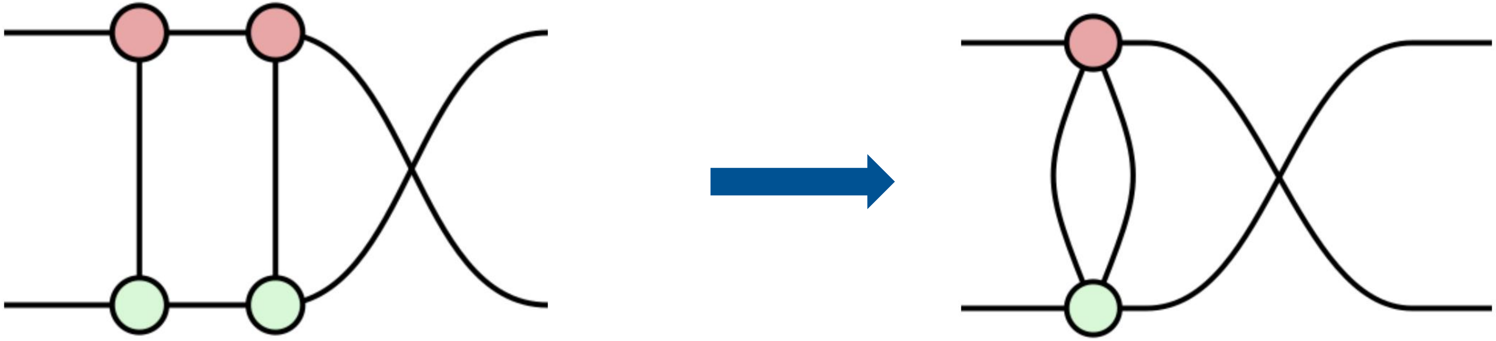
Simplification: Three CNOTs

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

Simplification: Three CNOTs

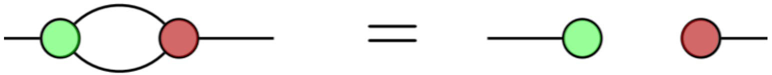


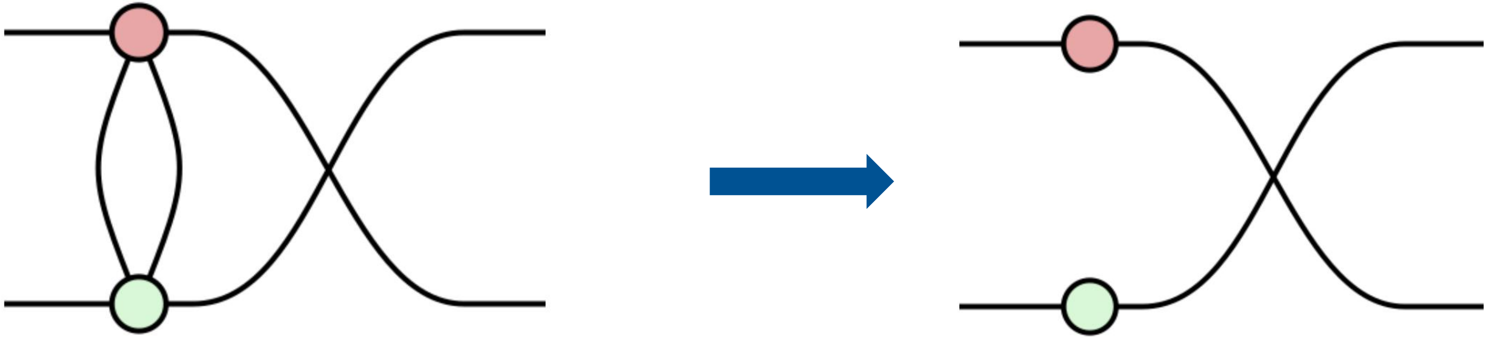
- Apply spider fusion rule
  - Attention, two wires remain between the first nodes!



Simplification: Three CNOTs

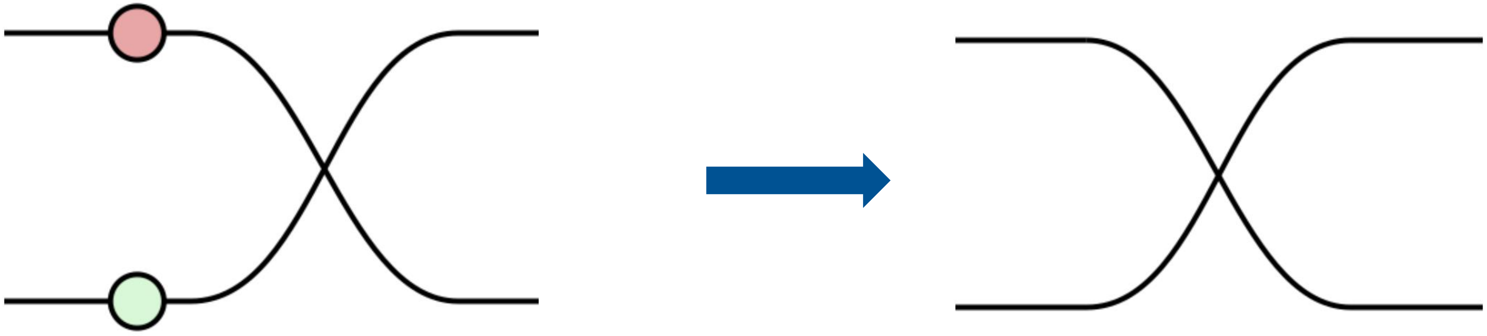
- Apply the Hopf-Law





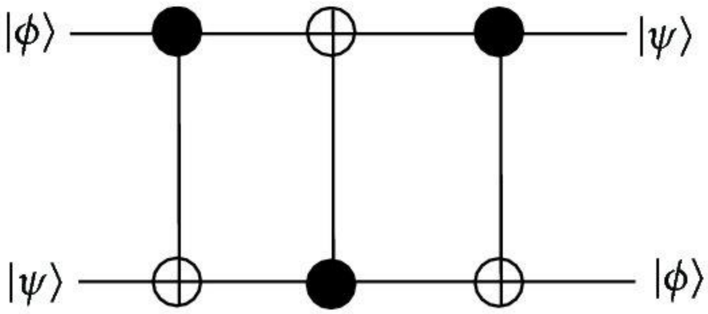
Simplification: Three CNOTs

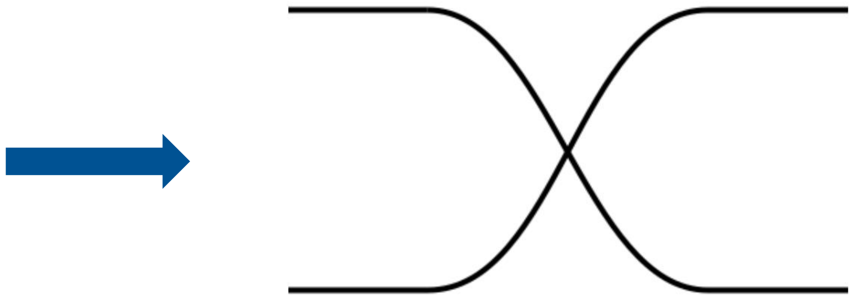
- Identity Removal



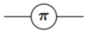
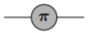
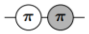
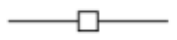
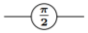
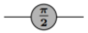
Simplification: Three CNOTs

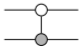
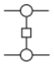
- Complicated CNOT circuit is actually a swap operation
  - Since we are working at the *atom*-level many other circuits can be simplified like this
  - Extracting back quantum circuits is hard
    - But it's possible for simple circuits
    - (In general: Graph needs to have “gFlow”)

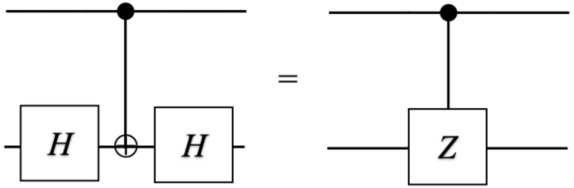




Translating Circuits

identity		$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
Pauli Z		$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
Pauli X NOT gate		$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Pauli Y	i 	$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
Hadamard gate		$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$
S gate		$\begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$
V gate		$\frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}$
T gate		$\begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$

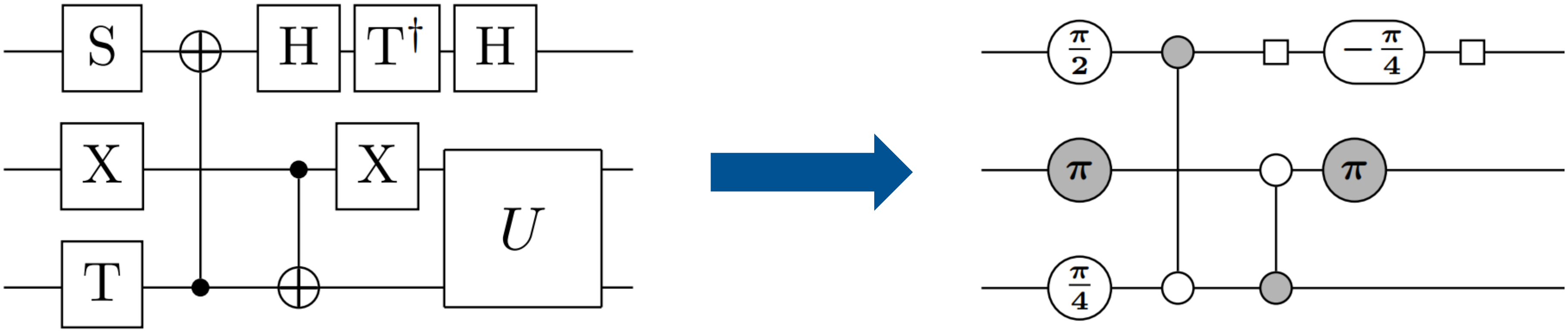
CNOT gate CX gate	$\sqrt{2}$ 	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
CZ gate	$\sqrt{2}$ 	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$



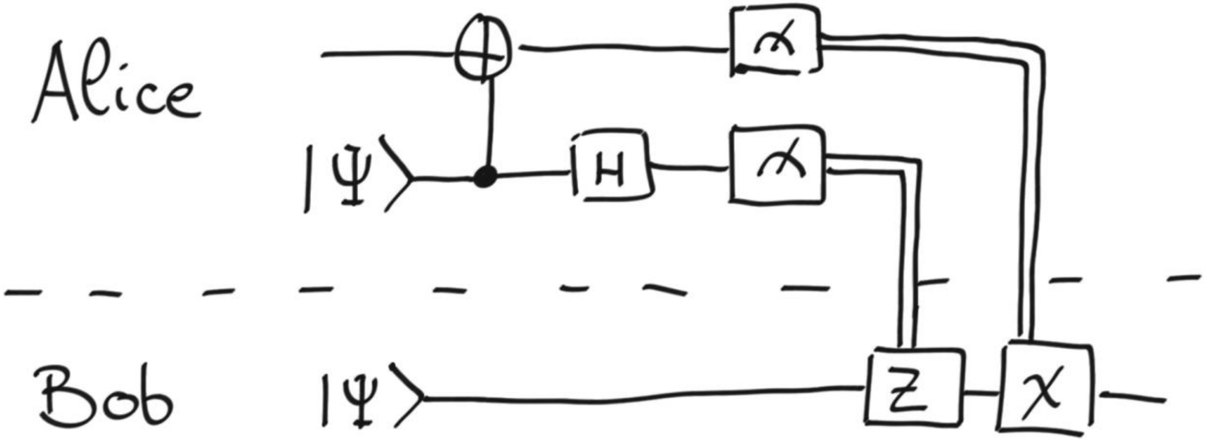
Challenge: Try to prove this identity!

From Quantum Circuits to ZX-Diagrams

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

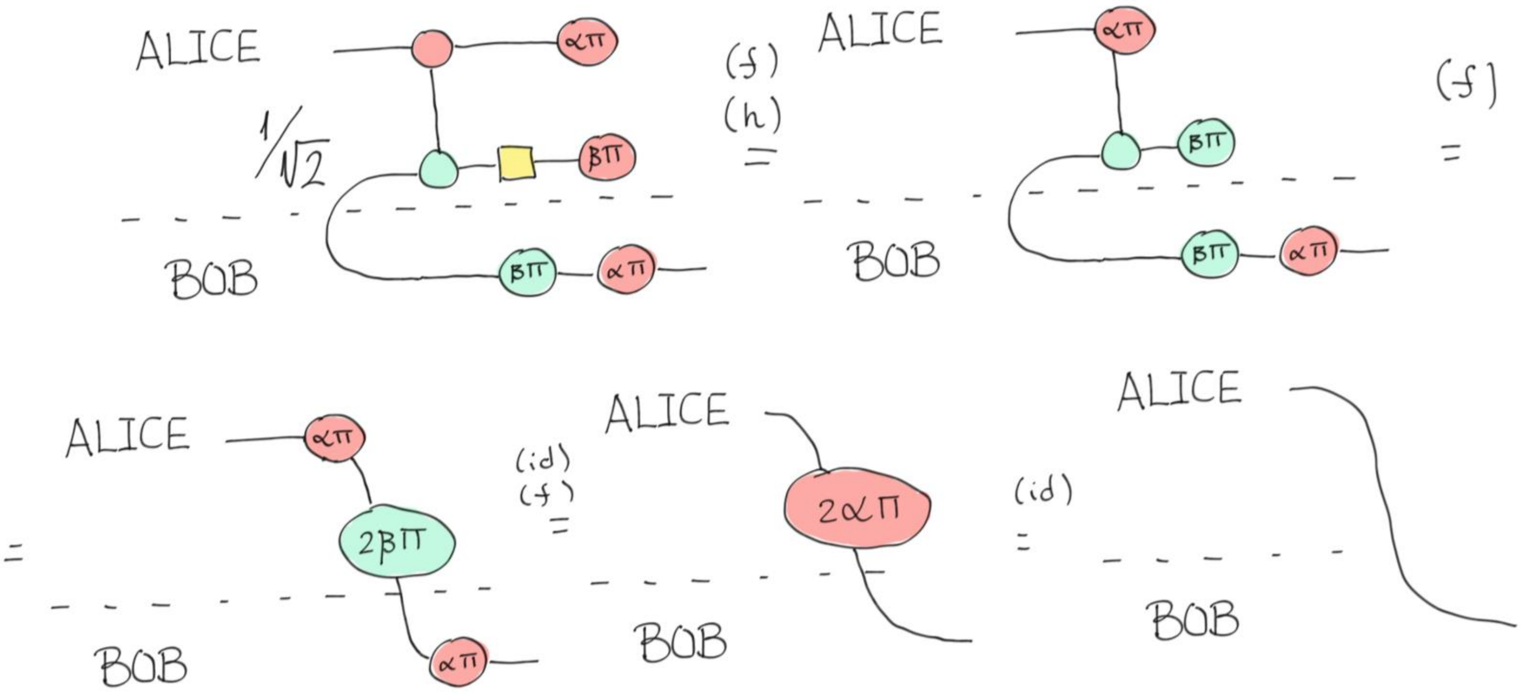


Quantum Teleportation



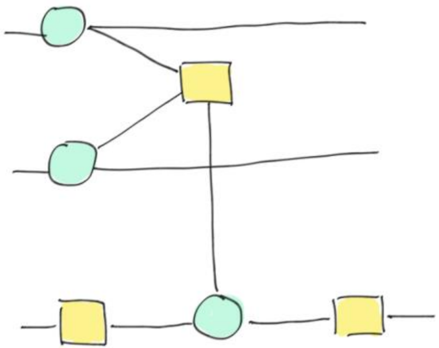
Quantum Teleportation

- Shared Bell State, is just a bent wire!



Toffoli Gate

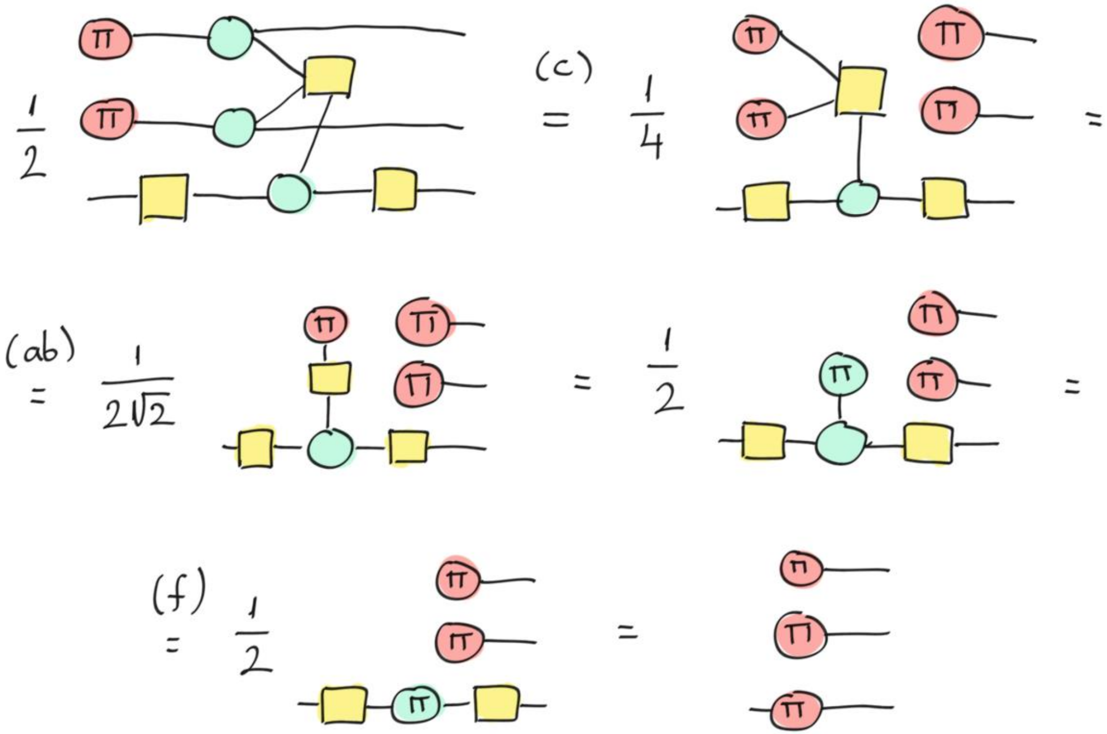
- Toffoli gate calculates a “quantum-AND” between two states
  - We introduced a new Generator: A “H-Box” to simplify the circuit. (Normally it has 25 Spiders)

$\frac{1}{2}$  $=$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

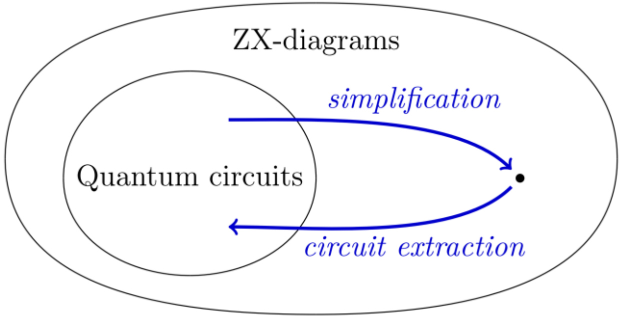
Toffoli Gate

- Toffoli Gate applied to $|11\rangle$



Completeness

- ZX Calculus is complete
  - Any two ZX-Graphs for the same Quantum circuit can be transformed into each other
  - By just using the rules from before!
- 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



Quellen

- Circuit compilation: https://www.cda.cit.tum.de/files/eda/2020_iscas_efficient_correct_compilation_quantum_circuits.pdf
  - https://quantum-journal.org/papers/q-2020-06-04-279/
- Mathematical Background https://www.youtube.com/watch?v=UQTTJV0ejfw
- Teleportation https://pennylane.ai/qml/demos/tutorial_zx_calculus

Images

- Circuit optimization P.4: https://quantum-journal.org/papers/q-2020-06-04-279/
- Spider Fusion P.33: https://www.cs.ox.ac.uk/people/bob.coecke/ZX-lectures_JPG.pdf