

Diagrammatic Design of Ansätze for Quantum Chemistry



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Pour ma mère et mon père.

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Summary

A central challenge in computational quantum chemistry is the accurate simulation of fermionic systems. At the heart of these calculations lies the need to solve the Schrödinger equation to determine the many-electron wavefunction. An exact solution to this problem scales exponentially with the number of electrons. Classical computers struggle to store the increasingly large wavefunctions making this problem computationally intractable in many cases. In contrast, gate-based quantum computing presents a promising solution, offering the potential to represent electronic wavefunctions with polynomially scaling resources [1]. In other words, quantum computers are a natural tool of choice for simulating processes that are inherently quantum [2].

In the last two decades many advancements in quantum computing have been made in both hardware and software bringing us closer to being able to simulate molecular systems. Despite these advancements, we remain in the so-called Noisy Intermediate Scale Quantum (NISQ) era, characterised by challenges such as poor qubit fidelity, low qubit connectivity and limited coherence times. The NISQ era represents a transitional phase in quantum computing, where quantum devices are not yet error-corrected but are still capable of performing computations beyond the reach of classical computers. Overcoming the limitations of the NISQ era is crucial for realising the full potential of quantum computing in various fields, including quantum chemistry and materials science.

The Variational Quantum Eigensolver (VQE) algorithm is a method used to estimate the ground state energy of a molecular Hamiltonian by preparing a trial wavefunction,

calculating its energy, and optimising the wavefunction parameters classically until the energy converges to the best approximation for the ground state energy [3]. It is recognised as a leading algorithm for quantum simulation on NISQ devices due to its reduced resource requirements in terms of qubit count and coherence time [4].

This thesis extends methods developed by Richie Yeung [2] for the preparation and analysis of parametrised quantum circuits, and applies them to ansätze representing fermionic wavefunctions. We are concerned with two main questions on this theme. Firstly, can we use the ZX calculus [cite] to gain insights into the structure of the unitary product ansatz in the context of variational algorithms for quantum chemistry? Secondly, in the context of NISQ devices, can we use these insights to build better ansätze with reduced circuit depth and more efficient resources?

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Chapter 1

Background

In this chapter, we will discuss the framework that we use to simulate fermionic systems on a quantum computer, as well as the notation that we will use throughout the text. Starting with Quantum Computation [REF\(quantum-computation\)](#) and Electronic Structure Theory [REF\(electronic-structure-theory\)](#), we will build up to unitary coupled cluster theory and the Variational Quantum Eigensolver [REF\(vqe\)](#).

Fermionic states can generally be represented on a quantum computer in the occupation number representation (section [REF\(second-quantisation\)](#)). That is, the state of each qubit is taken to represent the occupancy of each spin orbital. By representing the fermionic creation and annihilation operators in terms of qubit operators in a way that preserves the fermionic anticommutation relations, we can express the molecular Hamiltonian in terms of qubit operations.

Chapter 2

ZX Calculus

The ZX calculus is a diagrammatic language for reasoning about quantum processes
LALALA

2.1 Generators

By sequentially or horizontally composing the *Z Spider* (green) and *X Spider* (red) generators, we can construct undirected multigraphs known as ZX diagrams [5]. That is, graphs that allow multiple edges between vertices. Since *only connectivity matters* in the ZX calculus, a valid ZX diagram can be deformed as seen fit, provided that the order of inputs and outputs is preserved.

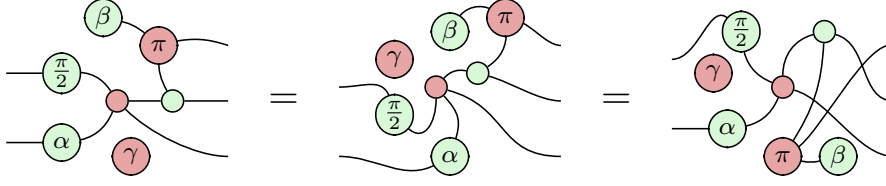


Figure 2.1: Three equivalent ZX diagrams (*only connectivity matters*).

Z Spiders are defined with respect to the *Z* eigenbasis such that a Z Spider with n inputs and m outputs has the following interpretation as a linear map. Note that in this text, we will interpret the flow of time from left to right.

$$n \begin{array}{c} \vdots \\ \text{---} \end{array} \begin{array}{c} \diagup \\ \text{---} \end{array} \begin{array}{c} \diagdown \\ \text{---} \end{array} m = |0\rangle^{\otimes m} \langle 0|^{\otimes n} + e^{i\alpha} |1\rangle^{\otimes m} \langle 1|^{\otimes n}$$

Figure 2.2: Interpretation of Z Spider as a linear map.

Similarly, X Spiders, which are defined with respect to the *X* eigenbasis, are interpreted as the following linear map.

$$n \begin{array}{c} \vdots \\ \text{---} \end{array} \begin{array}{c} \diagdown \\ \text{---} \end{array} \begin{array}{c} \diagup \\ \text{---} \end{array} m = |+\rangle^{\otimes m} \langle +|^{\otimes n} + e^{i\alpha} |-\rangle^{\otimes m} \langle -|^{\otimes n}$$

Figure 2.3: Interpretation of X Spider as a linear map.

We can recover the $|0\rangle$ eigenstate using an X Spider that has a phase of zero, or the $|1\rangle$ eigenstate using an X Spider that has a phase of π .

$$\text{---} \text{---} = |+\rangle + |-\rangle = \sqrt{2} |0\rangle$$

Figure 2.4: $|0\rangle$ eigenstate

$$\text{---} \text{---} = |+\rangle - |-\rangle = \sqrt{2} |1\rangle$$

Figure 2.5: $|1\rangle$ eigenstate

2. ZX Calculus

Likewise, we have the $|+\rangle$ and $|-\rangle$ basis states from the corresponding Z Spider

$$\text{---} \bigcirc \text{---} = |0\rangle + |1\rangle = \sqrt{2} |+\rangle \quad \text{---} \bigcirc^\pi \text{---} = |0\rangle - |1\rangle = \sqrt{2} |-\rangle$$

Figure 2.6: $|+\rangle$ eigenstate

Figure 2.7: $|-\rangle$ eigenstate

Whilst we obtain the correct states, we obtain the wrong scalar factor. For the remainder of this thesis, we will ignore global non-zero scalar factors. Hence, equal signs should be interpreted as ‘equal up to a global phase’.

Single qubit rotations in the Z basis are represented by a Z Spider with a single input and a single output. Arbitrary rotations in the X basis are represented by the corresponding X spider. We can view these as rotations of the Bloch sphere.

$$\begin{aligned} \text{---} \bigcirc^\alpha \text{---} &= |0\rangle\langle 0| + e^{i\alpha} |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\alpha} \end{pmatrix} \rightarrow \text{Bloch sphere with rotation around Z-axis} \\ \text{---} \bigcirc^\alpha \text{---} &= |+\rangle\langle +| + e^{i\alpha} |-\rangle\langle -| = \frac{1}{2} \begin{pmatrix} 1 + e^{i\alpha} & 1 - e^{i\alpha} \\ 1 - e^{i\alpha} & 1 + e^{i\alpha} \end{pmatrix} \rightarrow \text{Bloch sphere with rotation around X-axis} \end{aligned}$$

Figure 2.8: Arbitrary single qubit rotations in the Z and X bases.

We can recover the Pauli Z and Pauli X matrices by setting the angle $\alpha = \pi$.

$$\begin{aligned} \text{---} \bigcirc^\pi \text{---} &= |0\rangle\langle 0| + e^{i\pi} |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ \text{---} \bigcirc^\pi \text{---} &= |+\rangle\langle +| + e^{i\pi} |-\rangle\langle -| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

Figure 2.9: Pauli Z and X gates in the ZX calculus.

Composition

To calculate the matrix of a ZX diagram consisting of sequentially composed spiders, we take the matrix product. Note that the order of operation of matrix

2. ZX Calculus

multiplication is the reverse as in the ZX diagram as we have defined it.

$$\text{---} \circlearrowleft[\alpha] \text{---} \circlearrowright[\beta] \text{---} \circlearrowleft[\gamma] \text{---} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\gamma} \end{pmatrix} \begin{pmatrix} 1 + e^{i\beta} & 1 - e^{i\beta} \\ 1 - e^{i\beta} & 1 + e^{i\beta} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\alpha} \end{pmatrix}$$

Alternatively, we could have chosen to compose the spiders in parallel, resulting in the tensor product.

$$\begin{array}{c} \text{---} \circlearrowleft[\alpha] \text{---} \\ \text{---} \circlearrowright[\beta] \text{---} \end{array} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\alpha} \end{pmatrix} \otimes \begin{pmatrix} 1 + e^{i\beta} & 1 - e^{i\beta} \\ 1 - e^{i\beta} & 1 + e^{i\beta} \end{pmatrix}$$

The CNOT gate in the ZX calculus is represented by a Z spider (control qubit) and an X spider (target qubit). We can arbitrarily deform the diagram and decompose it into matrix and tensor products as follows.

$$\begin{array}{c} \text{---} \circlearrowleft \\ \text{---} \circlearrowright \end{array} = \begin{array}{c} \text{---} \circlearrowleft \\ \text{---} \circlearrowright \end{array} = \begin{array}{c} \boxed{A} \quad \boxed{B} \end{array}$$

We can calculate matrix A , consisting of a single-input and two-output Z Spider (4×2 matrix) and an empty wire (identity matrix), by taking the tensor product.

$$\boxed{A} = \begin{array}{c} \text{---} \circlearrowleft \\ \text{---} \end{array} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Similarly, to calculate the matrix B , we take the following tensor product.

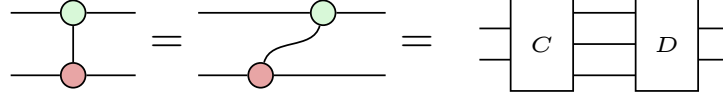
$$\boxed{B} = \begin{array}{c} \text{---} \\ \text{---} \circlearrowright \end{array} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

We can then calculate the CNOT matrix by taking the matrix product of matrix A and matrix B as follows.

$$\begin{array}{c} \text{---} \circlearrowleft \\ \text{---} \circlearrowright \end{array} = \left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \right] \left[\begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] \simeq \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

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Since *only connectivity matters* (2.1), we could have equivalently calculated the matrix of the CNOT gate by deforming the diagram as follows.



Had we chosen to make the first qubit the target and the second qubit the control, we would have obtained the following.

$$\begin{array}{c} \text{---} \text{red dot} \text{---} \\ | \\ \text{---} \text{green dot} \text{---} \end{array} = \left[\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] \left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix} \right] \simeq \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Hadamard Generator

All quantum gates are unitary transformations. Therefore, up to a global phase, an arbitrary single qubit rotation U can be viewed as a rotation of the Bloch sphere about some axis. We can decompose the unitary U using Euler angles to represent the rotation as three successive rotations [5].

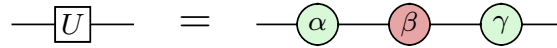


Figure 2.10: Arbitrary single-qubit rotation.

Recall that the Hadamard gate H switches between the $|0\rangle/|1\rangle$ and $|+\rangle/|-\rangle$ bases. That is, it corresponds to a rotation of the Bloch sphere π radians about the line bisecting the Z and X axes.

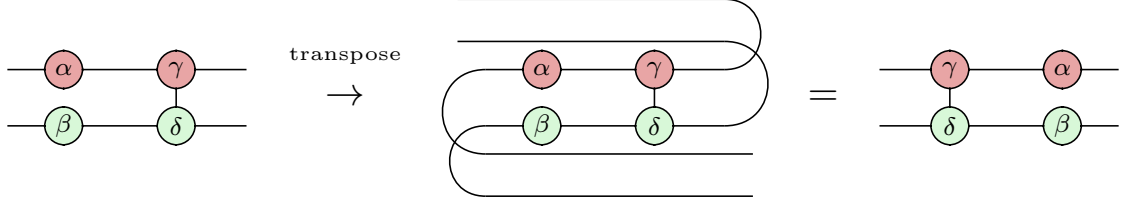
There are many equivalent ways of decomposing the Hadamard gate H using Euler angles. By choosing $\alpha = \beta = \gamma = \frac{\pi}{2}$, we obtain H up to a global phase of $\exp(-i\pi/4)$. See Appendix 4.2 for other definitions.

$$\text{---} \text{yellow square} \text{---} = e^{-i\frac{\pi}{4}} \text{---} \left(\text{green circle } \frac{\pi}{2} \right) \text{---} \left(\text{red circle } \frac{\pi}{2} \right) \text{---} \left(\text{green circle } \frac{\pi}{2} \right) \text{---} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

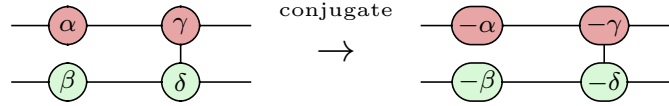
Figure 2.11: Definition of the Hadamard generator.

Conjugate, Transpose and Adjoint

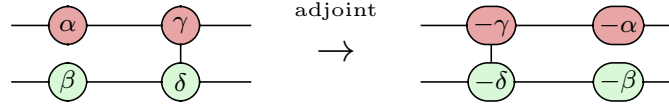
We can find the transpose of a ZX diagram by turning all of its inputs into outputs and all of its outputs into inputs whilst preserving the order of their wires.



We can find the conjugate of a ZX diagram by simply negating the phases of all spiders in the diagram, $\alpha \rightarrow -\alpha$, $\beta \rightarrow -\beta$, \dots .



It is then a simple matter to find the Hermitian adjoint of a ZX diagram by first finding its conjugate, then its transpose.



2.2 Rewrite Rules

This section introduces the various rewrite rules that come equipped with the ZX calculus. These rules extend the ZX calculus from notation into a language.

Spider Fusion

The most fundamental rule of the ZX calculus is the *spider fusion* rule [5]. It states that two spiders connected by one or more wires fuse if they are the same colour. It is the generalisation of adding the phases of successive rotations of the Bloch sphere. Since we interpret the phases α and β as $e^{i\alpha}$ and $e^{i\beta}$, it follows that the phase $\alpha + \beta$ is modulo 2π .

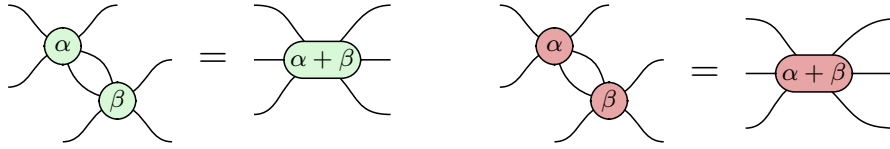


Figure 2.12: Spider fusion rule for Z spiders (left) and X spiders (right).

We can use this rule to identify commutation relations such as Z rotations commuting through CNOT controls, and X rotations, through CNOT targets.



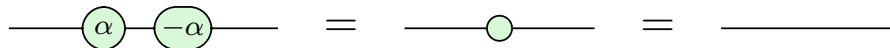
Identity Removal

The *identity removal* rule states that any two-legged spider with no phase ($\alpha = 0$) is equivalent to a rotation by 0 radians, or identity.



Figure 2.13: Identity removal rule.

Combining this with the spider fusion rule (2.12), we see that two successive rotations with opposite phases is equivalent to an empty wire.



2. ZX Calculus

π Copy Rule

The π *copy* rule concerns itself with the interactions of the Pauli Z and X gates with spiders. It states that when a Pauli Z or Pauli X gate is pushed through a spider of the opposite colour, it copies through the spider and flips its phase.

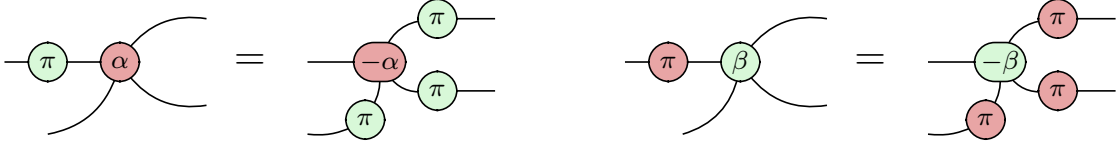


Figure 2.14: π copy rule for Z and X spiders.

State Copy Rule

A similar rule derived from the π copy rule (2.14), is the *state copy* rule. It states that the $|0\rangle$ state (phaseless X spider) and the $|1\rangle$ state (X spider with phase π) interact with Z spiders as follows. The same rule holds for the colour-flipped counterparts.



Figure 2.15: State copy rule for the X eigenstates.

Bialgebra Rule

Unlike the previous rules we have introduced, the *bialgebra rule* takes some time to understand intuitively. It is nevertheless important in many derivations. We can represent the eigenstates of the X and Z operators by introducing the boolean variable $a \in \{0, 1\}$ as follows.

$$\text{red circle with } a\pi \text{ ---} = |0\rangle \text{ where } a = 0 \text{ and } |1\rangle \text{ where } a = 1$$

$$\text{green circle with } a\pi \text{ ---} = |+\rangle \text{ where } a = 0 \text{ and } |-\rangle \text{ where } a = 1$$

Using the spider fusion rule (2.12), we are able to show that an X spider with two inputs and one output behaves like the classical XOR gate when applied to the $|0\rangle$

2. ZX Calculus

and $|1\rangle$ states. Using the state copy rule (2.15), we are able to show that a Z spider with one input and two outputs behaves like the classical COPY gate.



Figure 2.16: X spider as a XOR gate (left) and Z spider as a COPY gate (right).

Let us now consider the natural commutation relation of the classical XOR and COPY gates. It is clear that XORing two bits then copying them is the same as copying the same two bits, then XORing them. Using this relation as motivation, we define the *bialgebra* rule.

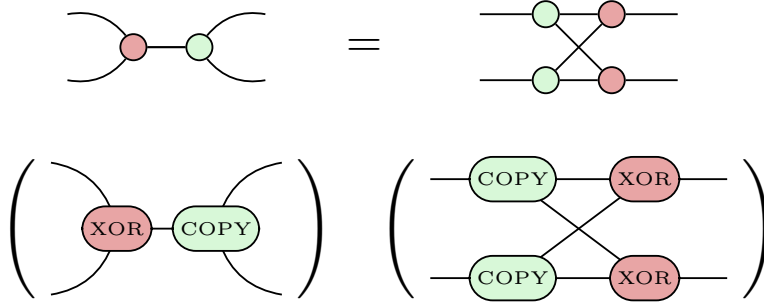


Figure 2.17: The bialgebra rule (top) and its classical motivation (bottom).

The bialgebra rule is then the quantum generalisation of the XOR-COPY commutation relation. It holds for all states, not just the computational basis states.

Hopf Rule

Finally, we have the Hopf rule, which states that we can remove the wires connecting an X spider and a Z spider when the number of connections between them is two. Like with the bialgebra rule (2.17), we can take motivation from the behaviour of the classical XOR and COPY gates, since COPYING two bits then XORing them always yields 0.

2. ZX Calculus

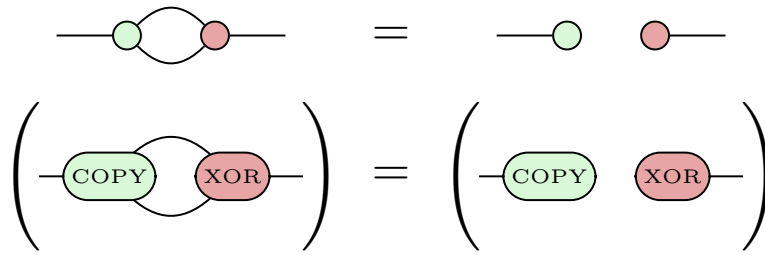


Figure 2.18: The Hopf rule (top) and its classical motivation (bottom).

Chapter 3

Pauli Gadgets

Pauli gadgets form the building blocks for ansätze for quantum chemical simulations. We will see in chapter XXX how they can be used to construct excitation operators to ultimately calculate electronic correlation in a molecular system.

3.1 Phase Gadgets

Missing: matrix representation

Phase gadgets are a special type of Pauli gadget formed from Pauli strings consisting of the Pauli I and Z matrices. A Pauli string P is defined as a tensor product of Pauli matrices $P \in \{I, Y, Z, X\}^{\otimes n}$, where n is the number of qubits in the system. each Pauli operator acts on a distinct qubit. Note that since the Pauli matrices are Hermitian, so are Pauli strings. Thus $Z \otimes Y \otimes X = ZYX$ means apply Pauli Z , Y and X to qubits 0, 1 and 2 respectively.

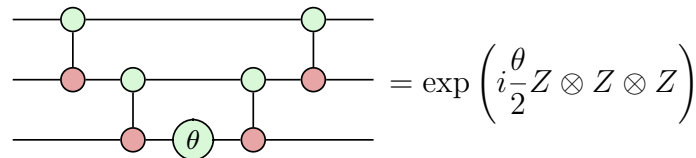
Stone's Theorem [6] states that a strongly continuous one parameter unitary group $U(\theta)$ is generated by a Hermitian operator, P .

$$U(\theta) = \exp\left(i\frac{\theta}{2}P\right) \quad \text{where} \quad e^X = 1 + X + \frac{1}{2}X^2 + \frac{1}{6}X^3 + \dots$$

There is therefore a one-to-one correspondence between Hermitian operators and one parameter unitary groups [2]. The time evolution of a quantum mechanical system, described by the Hamiltonian H , is defined by the one parameter unitary group e^{itH} , whilst arbitrary rotation gates in the Z , X and Y bases are described by the one parameter unitary groups of the Pauli matrices Z , X and Y .

$$R_Z(\theta) = \exp\left(i\frac{\theta}{2}Z\right) \quad R_Y(\theta) = \exp\left(i\frac{\theta}{2}Y\right) \quad R_X(\theta) = \exp\left(i\frac{\theta}{2}X\right)$$

Phase gadgets are defined as the one parameter unitary groups of Pauli strings consisting of the I and Z matrices, $P \in \{I, Z\}^{\otimes n}$. They correspond to quantum circuits made up of a Z rotation wedged between two CNOT layers.



The first CNOT layer can be thought of as computing the parity of the input state by entangling the qubits. The Z rotation then rotates the entangled state by $e^{i\theta/2}$ or $e^{-i\theta/2}$, depending on the parity of the state, and the final CNOT layer

3. Pauli Gadgets

uncomputes the parity. Phase gadgets necessarily correspond to diagonal unitary matrices in the Z basis since they apply a global phase to a given state without changing the distribution of the observed state [2]. This diagonal action suggests that a symmetric ZX diagram exists for phase gadgets, as is indeed the case.

$$\begin{array}{c} \text{Circuit 1} \end{array} = \begin{array}{c} \text{Circuit 2} \end{array} = \exp\left(i\frac{\theta}{2}Z \otimes Z \otimes Z\right)$$

By deforming d our phase gadget in quantum circuit notation and using the identity id (2.13), spider fusion f (2.12) and bialgebra ba (2.17) rules, we are able to show the correspondence with its form in the ZX calculus.

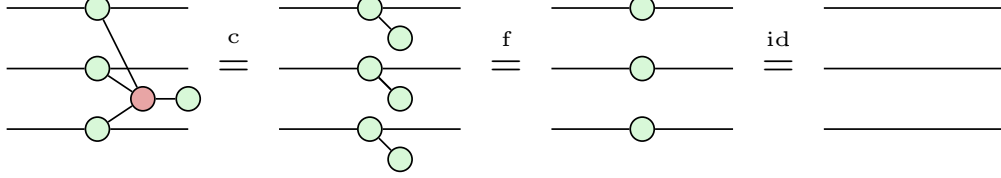
It is then a simple matter of recursively applying this proof to phase gadgets in quantum circuit notation to generalise to arbitrary arity.

Not only is this representation intuitively self-transpose, but it comes equipped with various rules describing its interaction with other phase gadgets and quantum gates.

3. Pauli Gadgets

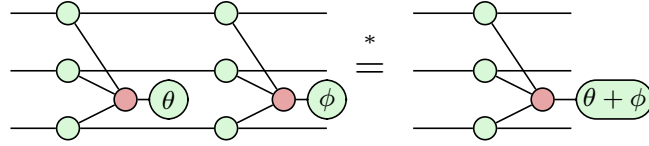
Phase Gadget Identity Rule

Phase gadgets with an angle $\theta = 0$ can be shown to be equivalent to identity using the state copy (2.15), spider fusion (2.12) and identity removal (2.13) rules.



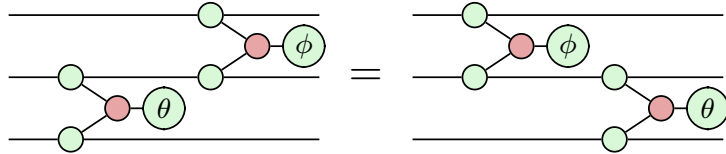
Phase Gadget Fusion Rule

Any two adjacent phase gadgets formed from the same Pauli string fuse and their phases add. This is achieved using the spider fusion rule (2.12) and the bialgebra rule (2.17). See Appendix 4.2 for the intermediate steps marked (*).



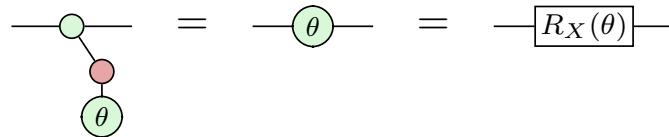
Phase Gadget Commutation Rule

Any two adjacent phase gadgets commute, as can be shown using the spider fusion rule 2.12 (fuse then unfuse the legs 2.12).



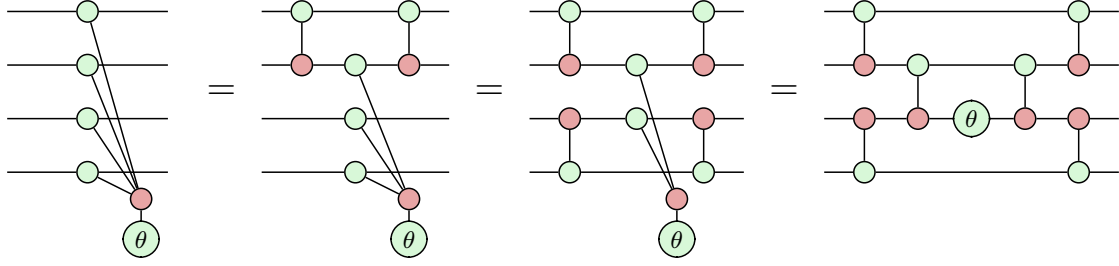
Single-Legged Phase Gadgets

Single-legged phase gadgets are equivalent to Z rotations. See the proof in Appendix 4.2.



Phase Gadget Decomposition

There are many equivalent ways of decomposing a phase gadget into quantum circuit notation using the bialgebra rule (2.17). More generally, we can show that it is possible to decompose a phase gadget such that it has a circuit depth of $\log_2(n)$ instead of n , where n is the number of qubits.



Clearly, it is then advantageous to manipulate circuits of phase gadgets using the ZX calculus, and to extract the corresponding quantum circuit only after the ZX diagram has been optimised.

3.2 Pauli Gadgets

Pauli gadgets are defined as the one parameter unitary groups of Pauli strings consisting of all four Pauli matrices, $P \in \{I, Z, X, Y\}$. They are essentially phase gadgets associated with an additional change of basis.

$$= \exp\left(i\frac{\theta}{2}Y \otimes Z \otimes X\right)$$

Whilst phase gadgets alone cannot change the distribution of the observed state, Pauli gadgets, which are associated with a change of basis, can [2]. We will later see how Pauli gadgets form the building blocks in ansätze used for quantum chemical simulations. Similarly to phase gadgets, Pauli gadgets come equipped with a set of rules describing their interactions with other gadgets and quantum gates.

Pauli Gadget Identity Rule

Pauli gadgets with an angle $\theta = 0$, and matching legs, can be shown to be equivalent to identity using the phase gadget identity rule (3.1), and the subsequent cancellation of the change of basis layers.

$$= \text{Identity}$$

Pauli Gadget Fusion Rule

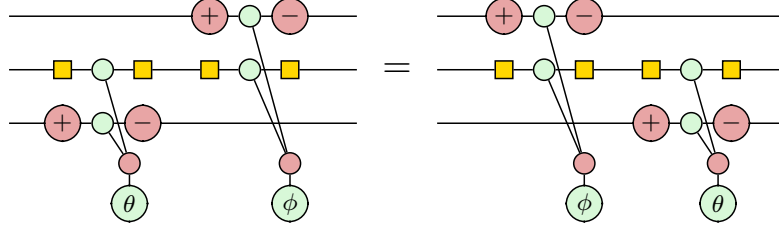
Likewise, any two adjacent Pauli gadgets with matching legs fuse and their phases add. This is achieved by cancelling adjacent change of basis layers and using the phase gadget fusion rule (3.1).

$$= \text{Fused Gadget with phase } \theta + \phi$$

3. Pauli Gadgets

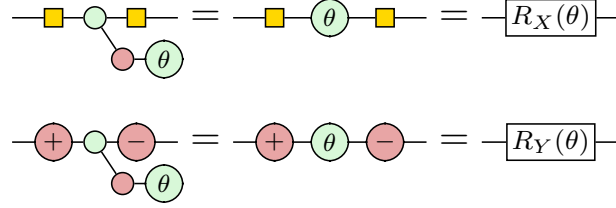
Pauli Gadget Commutation Rule

Any two adjacent Pauli gadgets with no mismatching legs can be shown to commute. This is achieved by cancelling adjacent change of basis layers, and using the spider fusion rule (fuse then unfuse the legs 2.12).



Single-Legged Pauli Gadgets

Finally, we can show that single-legged Pauli gadgets are equivalent to a rotation in the corresponding basis using the single-legged phase gadget rule (3.1).



Chapter 4

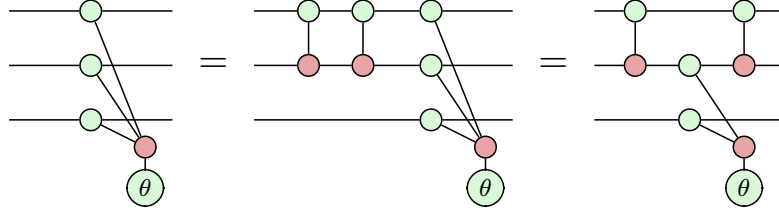
Commutation Relations

In this chapter, we will develop a set of rules to describe the interaction of Pauli gadgets with other Pauli gadgets, CNOT gates and Clifford gates. We will refer to these rules as *commutation relations*. Note, we are not referring to the quantum mechanical definition of commutation, but rather, what happens to two ZX diagrams when pushed through one another.

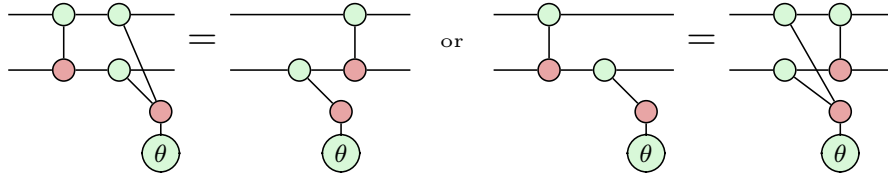
4. Commutation Relations

4.1 CNOT Commutation

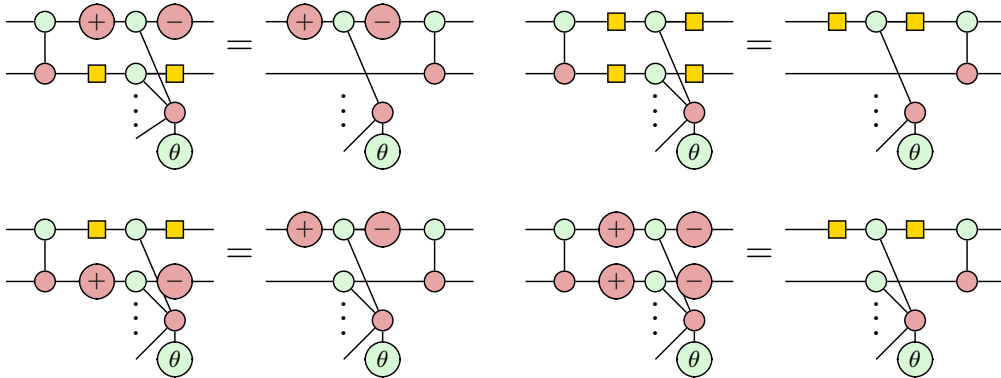
When a CNOT gate is *pushed* through a Pauli gadget, it modifies the gadget's legs. That is, the resulting gadget is defined by a new Pauli string. We have encountered when using the bialgebra rule (2.17) to construct phase gadgets 3.1.



Above, we have inserted two adjacent CNOTs (self-inverse), then pushed one of them through the phase gadget. We can say that a CNOT gate ‘commutes’ through a $\exp[i\frac{\theta}{2}(Z \otimes Z)]$ gadget to get a $\exp[i\frac{\theta}{2}(I \otimes Z)]$ gadget.



The ZX calculus can be used to identify how CNOT gates commute through any Pauli gadget. Note that the following examples are not exhaustive – there are 16 possible permutations with repetition of $\{I, X, Y, Z\}$ taken two at a time.)



In practice, it may be tedious to use the bialgebra and other rules to identify each commutation relation. There exists, however, a simple trick for identifying these relations. The CNOT gate belongs to the Clifford group C . That is, the set of

4. Commutation Relations

transformations that normalise the Pauli group. For instance, conjugating the Pauli X gate with the Hadamard H (where $H \in C$), yields the Z gate.

$$Z = HXH$$

Recall that Pauli gadgets are defined as one parameter unitary groups of a given Pauli string P , where $P \in \{I, Z, X, Y\}^{\otimes n}$. It can be shown, through the relevant Taylor expansion, that conjugating a Pauli gadget is equivalent to finding the one parameter unitary group of the conjugated Pauli string (see Appendix 4.2).

4. Commutation Relations

4.2 Clifford Commutation

Appendices

Hadamard

Below are several equivalent definitions of the Hadamard generator. Note that the two rightmost definitions do not require any scalar correction.

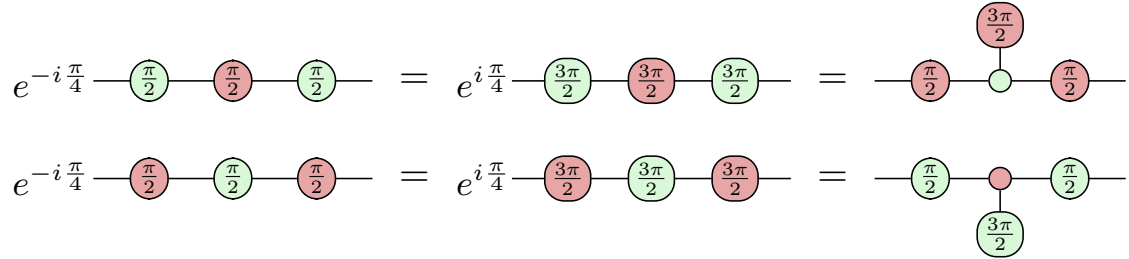
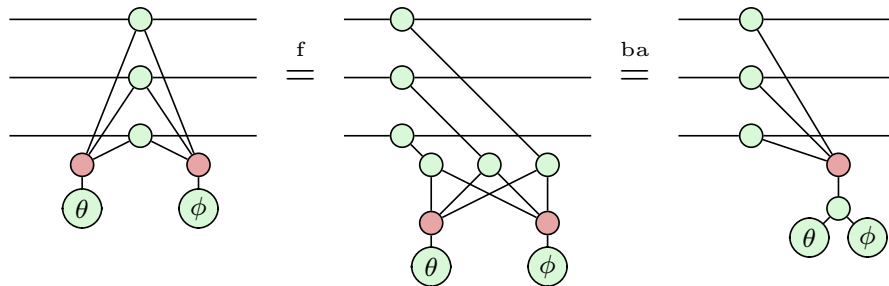


Figure 1: Equivalent definitions of the Hadamard generator.

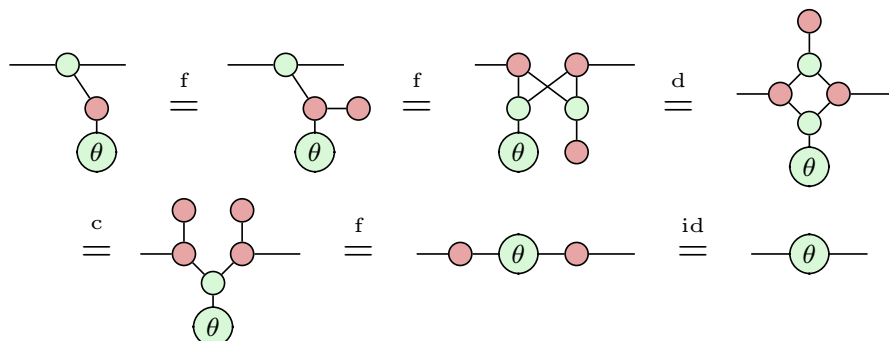
Phase Gadgets

We can show how two adjacent phase gadgets fuse using the spider fusion (2.12) and bialgebra (2.17) rules as follows.



Single-Legged Phase Gadgets

We can show that single-legged phase gadgets are equivalent to Z rotations using the bialgebra (2.17), spider fusion (2.12), state copy (2.15) and identity (2.13) rules as follows.



Clifford Conjugation Stuff

$$C e^P C^\dagger = C \sum_{n=0}^{\infty} \left(\frac{P^n}{n!} \right) C^\dagger$$

$$C P^n C^\dagger = \sum_{n=0}^{\infty} \frac{C P^n C^\dagger}{n!}$$

$$C P^n C^\dagger = \sum_{n=0}^{\infty} \frac{(C P C^\dagger)^n}{n!}$$

$$C P^n C^\dagger = (C P C^\dagger)^n$$

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