Measurement-Based Variational Quantum Eigensolver

(MB-VQE)

QLOC Talk – Journal Club
Quantum and Linear Optical Computation (QLOC) Group

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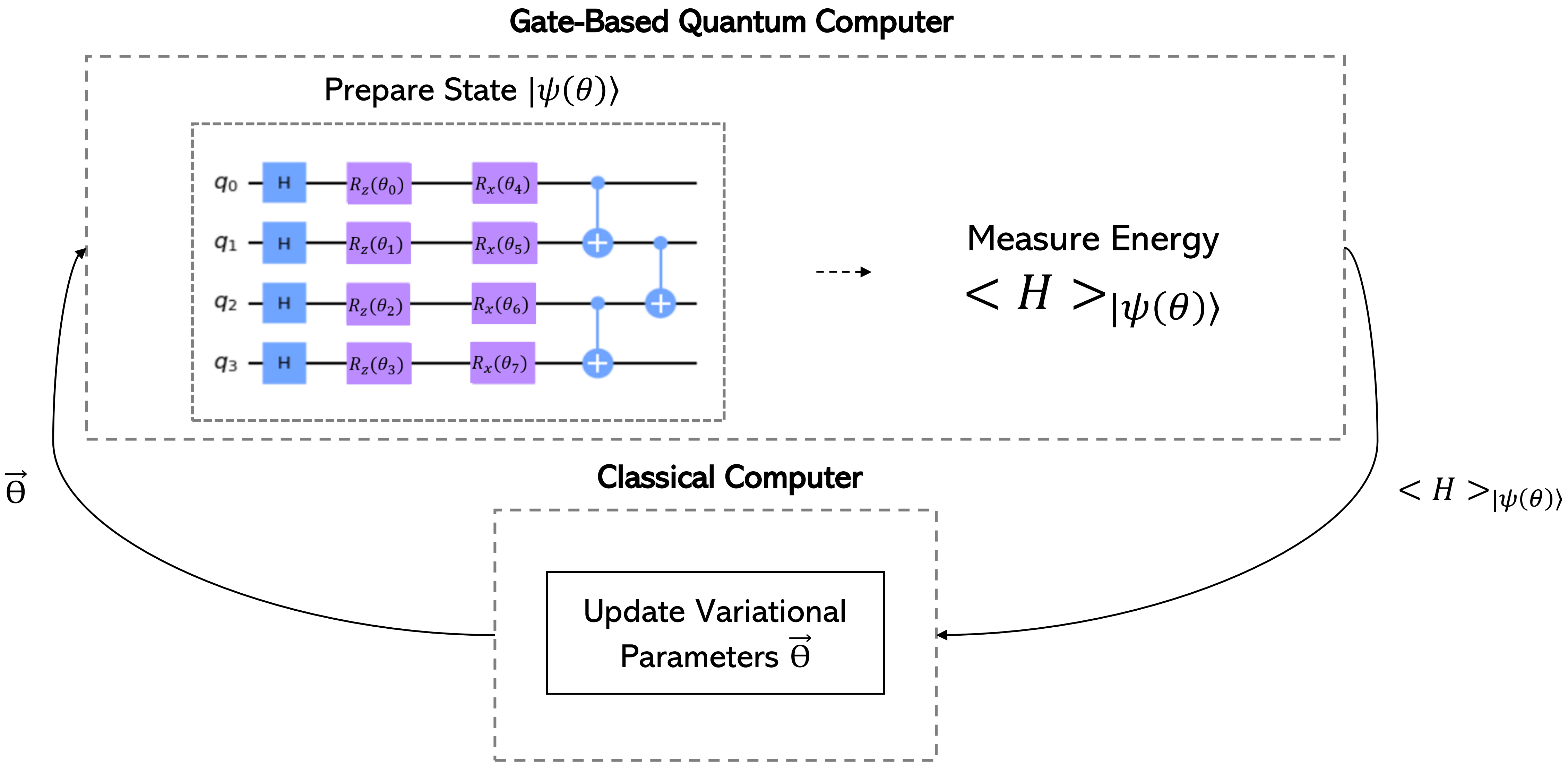
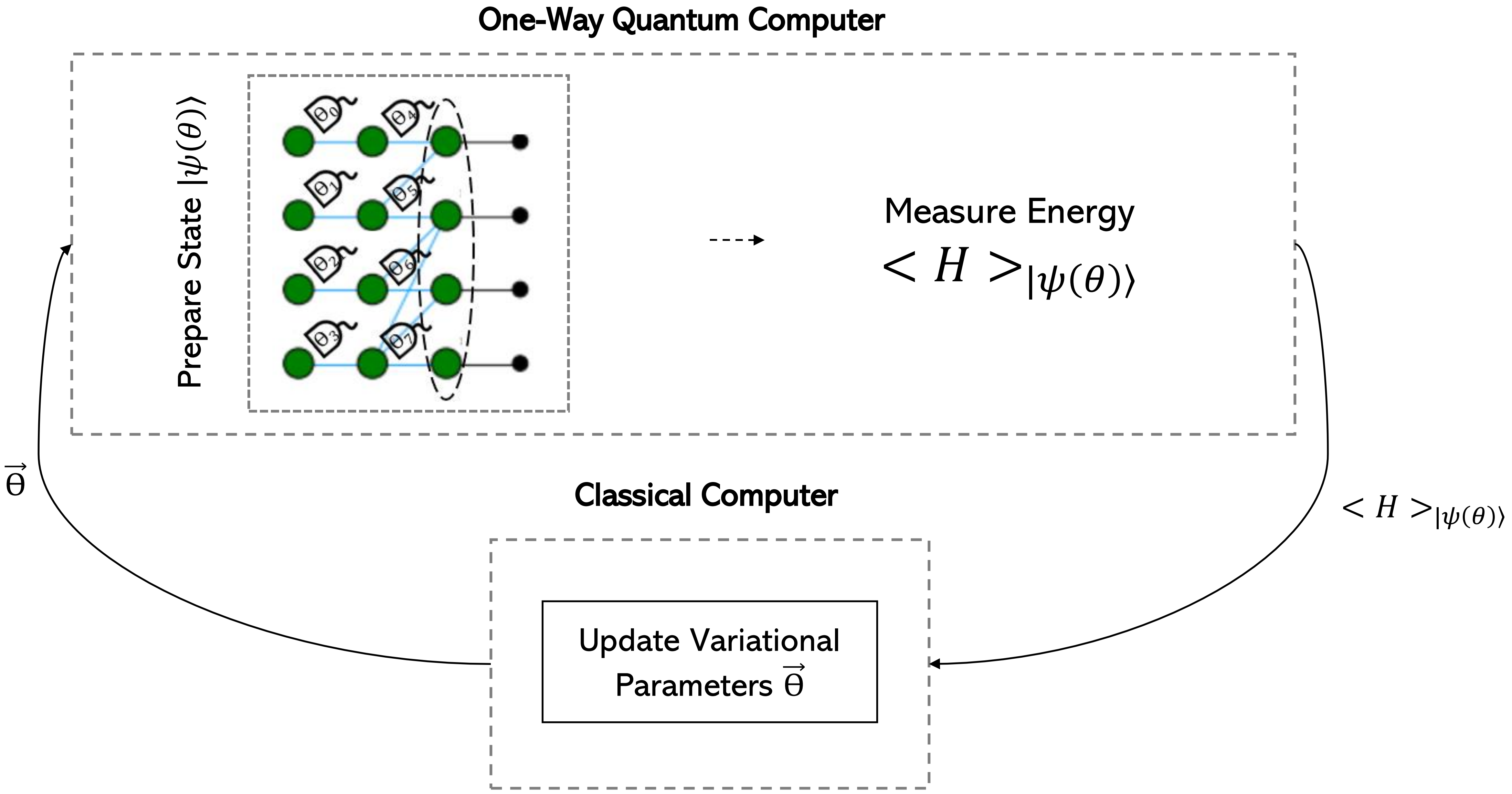
Circuit Model VQE



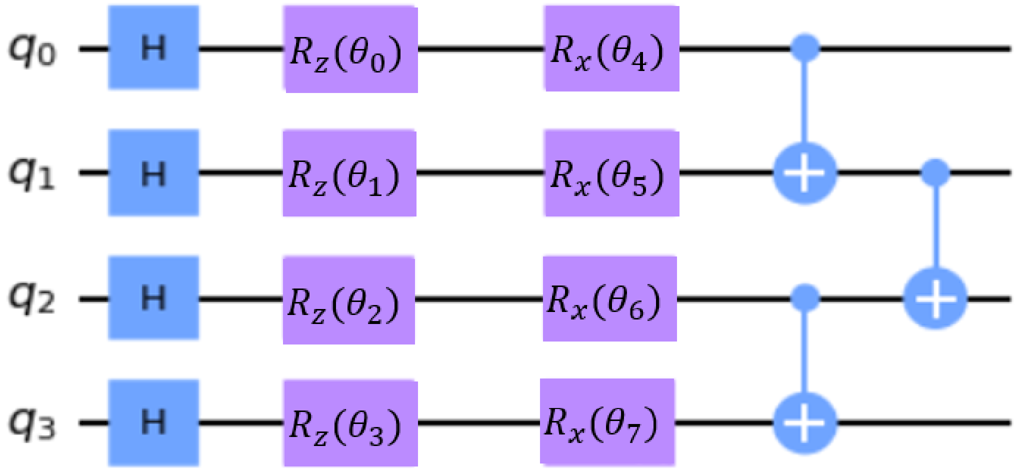
(Peruzzo et al., 2014)

Measurement-Based VQE



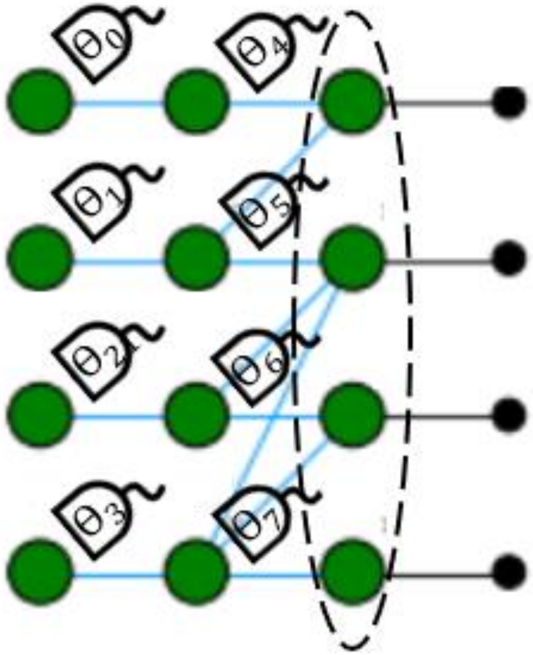
(Ferguson et al., 2021)

CM-VQE



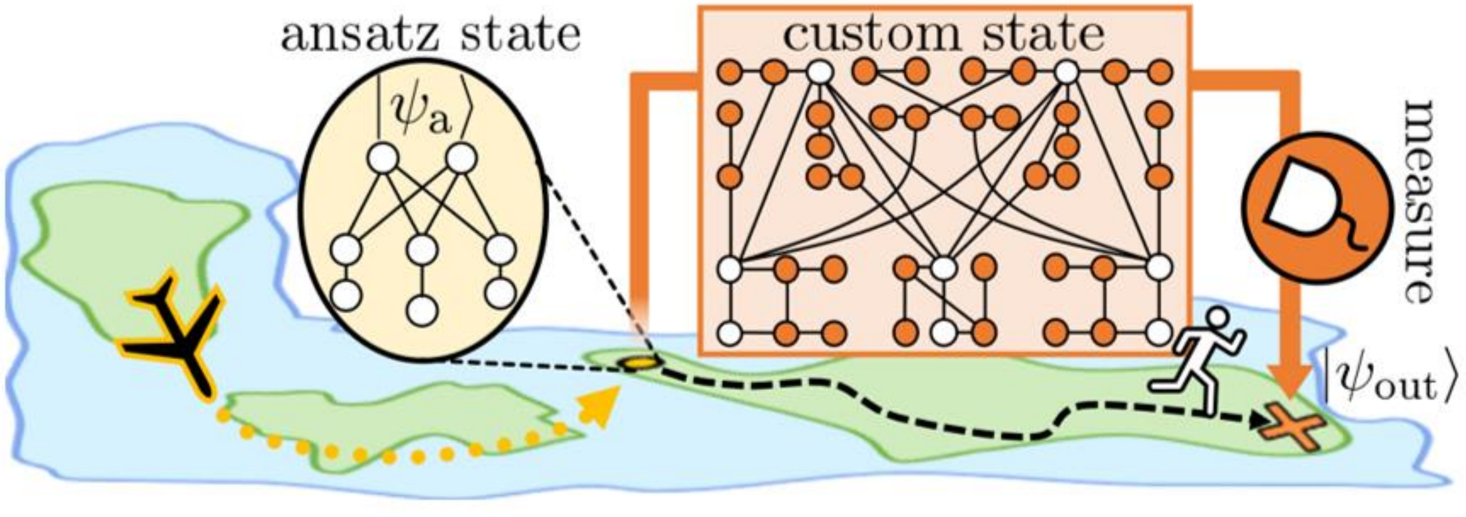
- Variational state is prepared by applying gates on the all-zero state
- Reference state preparation and application of $U(\vec{\theta})$ correspond to portions of the circuit
- $\vec{\theta}$ are gate parameters

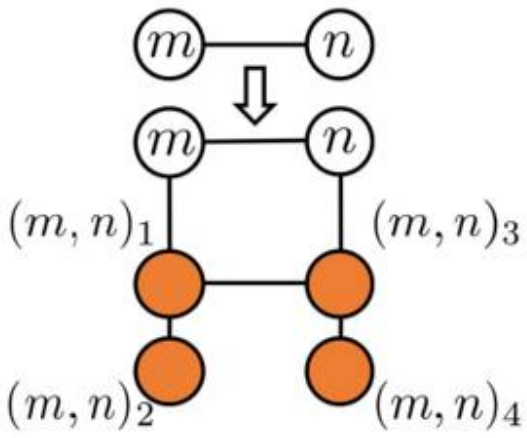
MB-VQE



- Variational state is prepared by creating an entangled resource state and measuring the ancillae
- Reference state preparation and application of $U(\vec{\theta})$ correspond to portions of the graph state
- $\vec{\theta}$ are angles of measurement bases for ancilla qubits

Option I: Edge Decoration of a Problem-Specific Ansatz

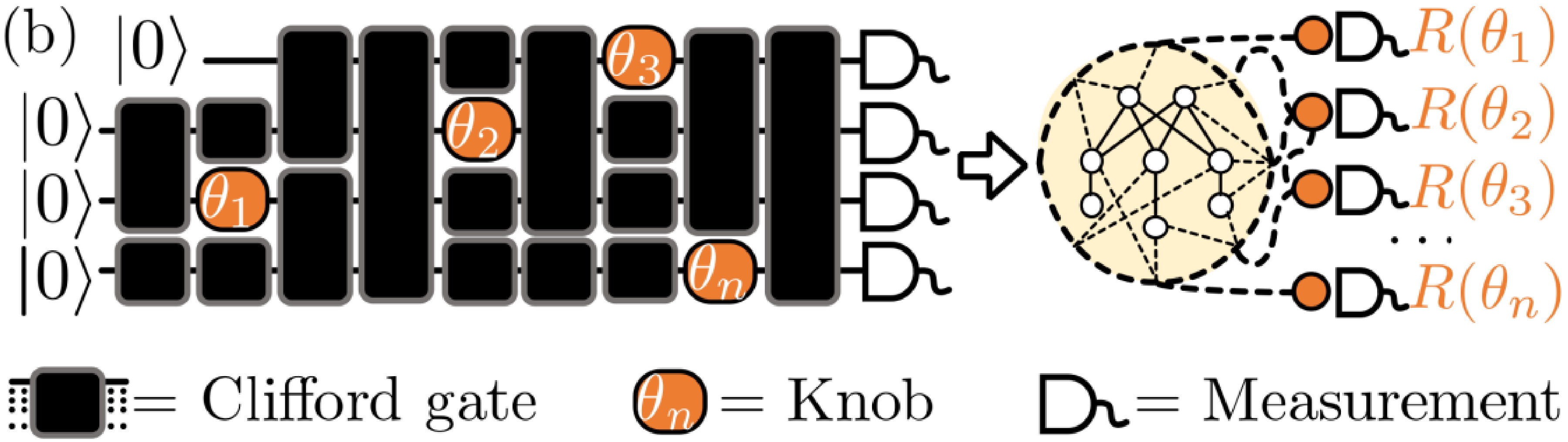




- Ancilla qubits are added to a problem-specific graph state with the intent of producing parameterized modifications
- No direct circuit-model analogue to the transformations caused by measuring the ancillae
- Example use case: a perturbation is added to a Hamiltonian whose (known) ground state is a stabilizer state

(Ferguson et al., 2021)

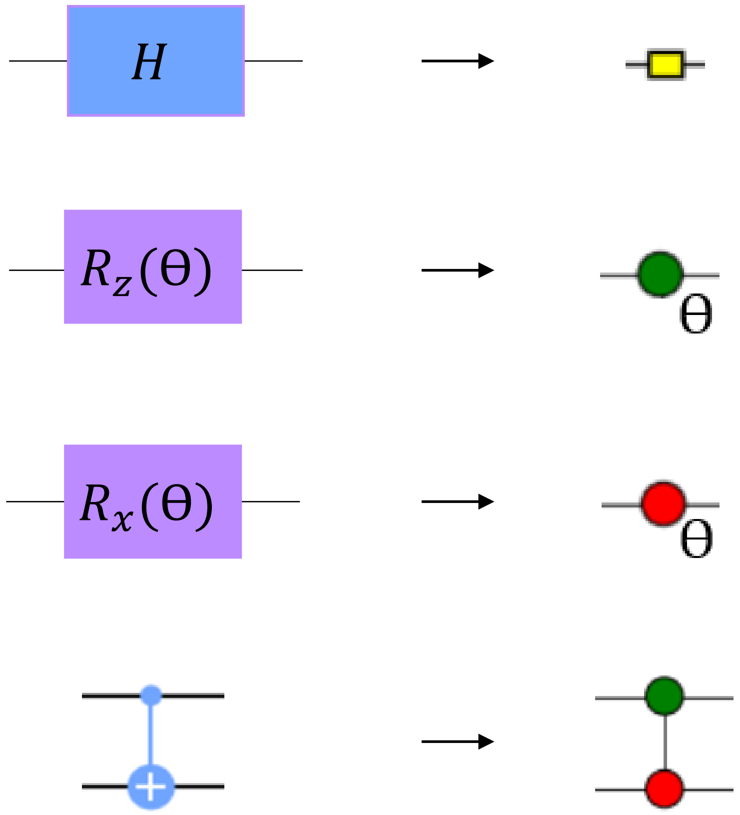
Option II: Direct Translation from Circuit Model VQE

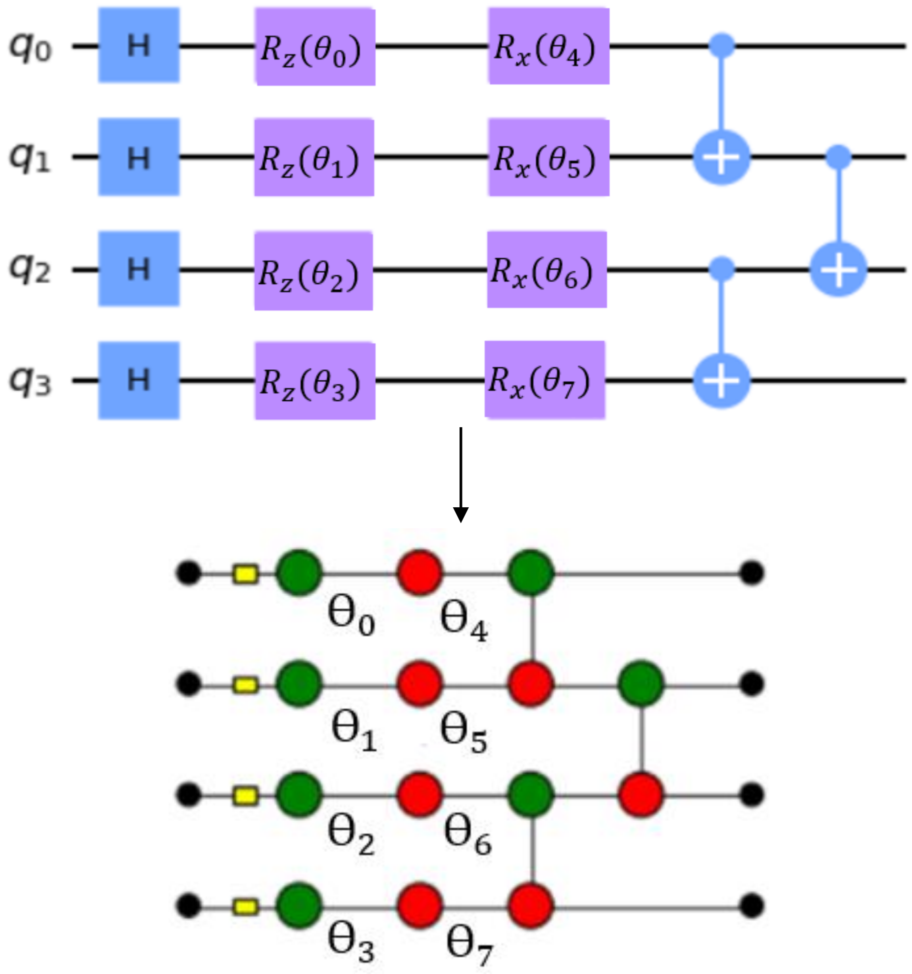


- Translate a variational circuit to a measurement protocol on a graph state
- Same achievable states: search space is left unchanged
- Example use case: platform favours preparation of entangled states over application of entangling gates

(Ferguson et al., 2021)

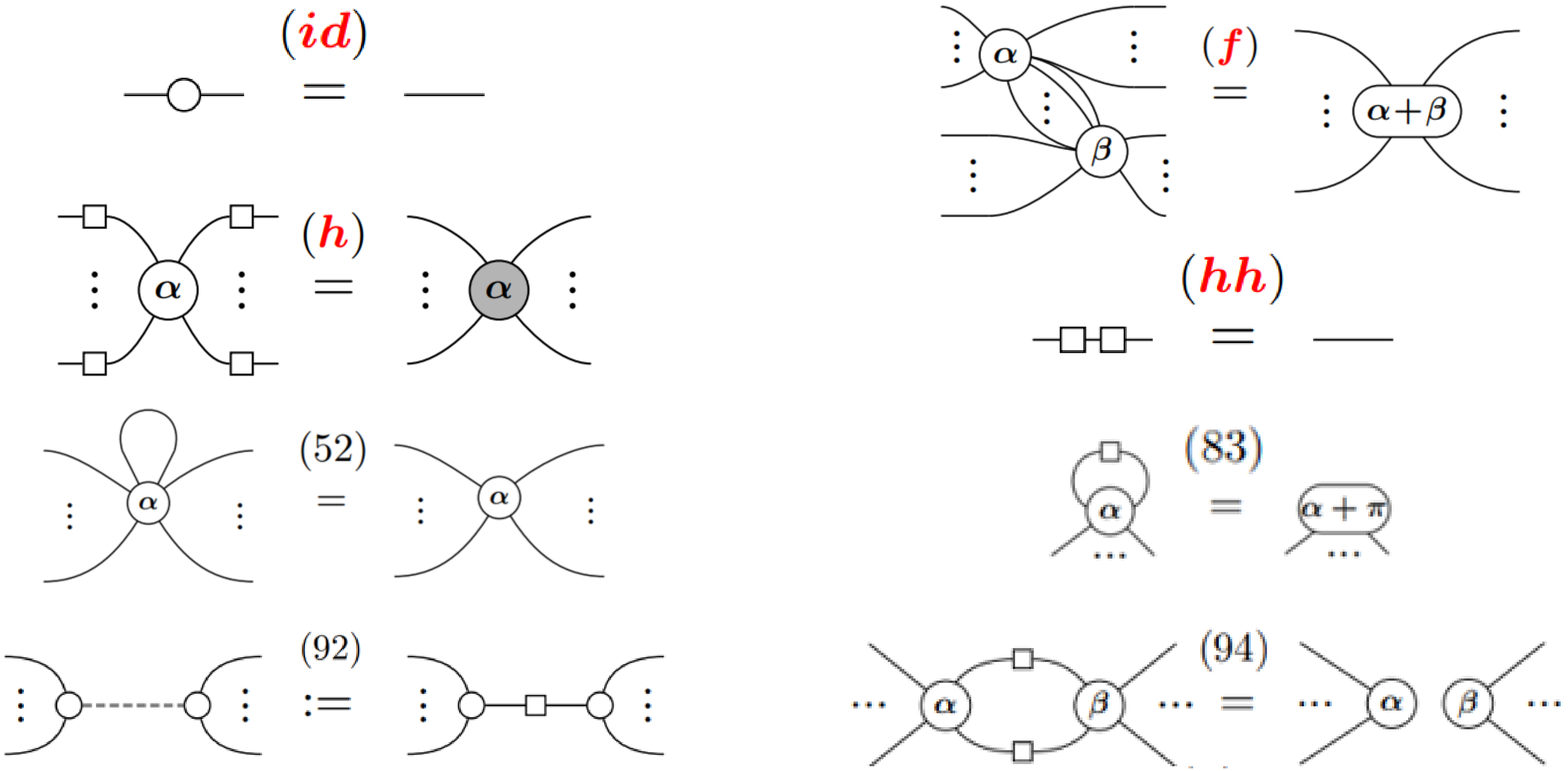
From Circuits to ZX-Diagrams





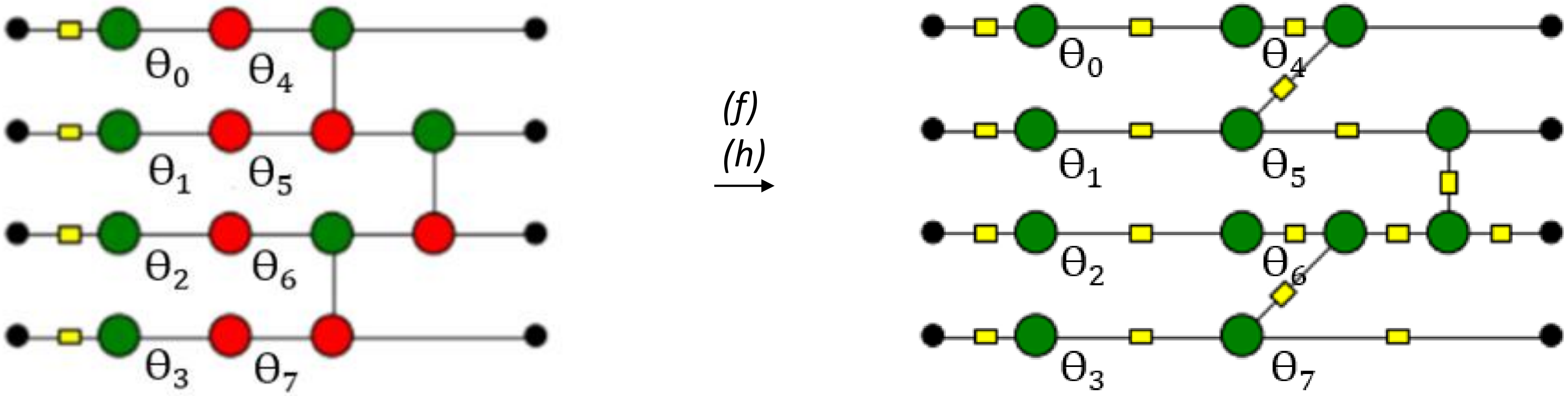
(van de Wetering, 2020)
(Kissinger, 2020)

From ZX-Diagrams to Graph-Like ZX-Diagrams

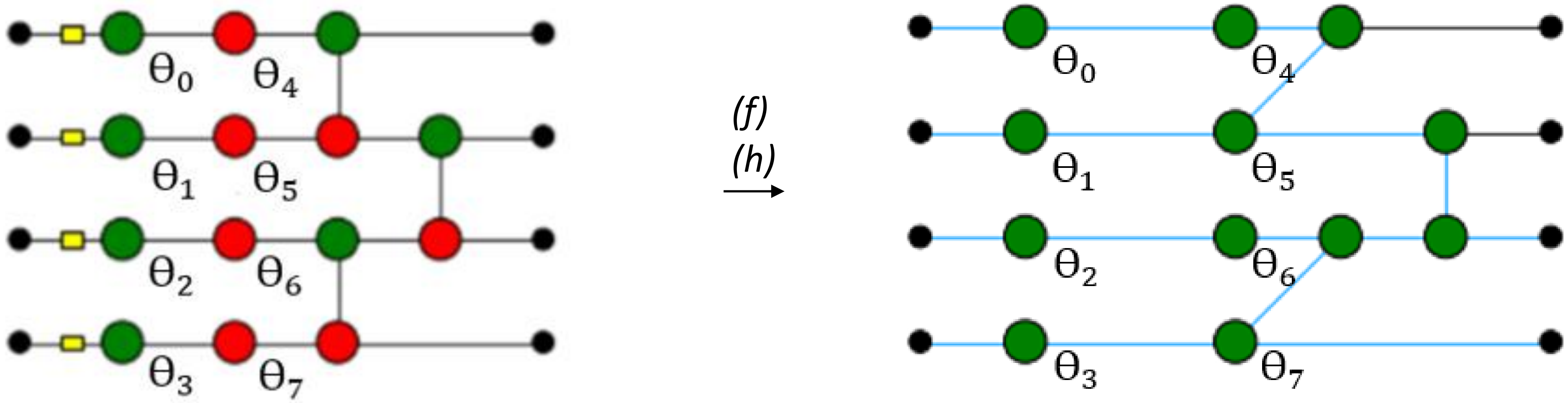


Using (id), (f), (h), (hh), (52), (83), (92), (94), we can transform any ZX diagram into a graph-like ZX diagram. These diagrams represent graph states.

From ZX-Diagrams to Graph-Like ZX-Diagrams



From ZX-Diagrams to Graph-Like ZX-Diagrams



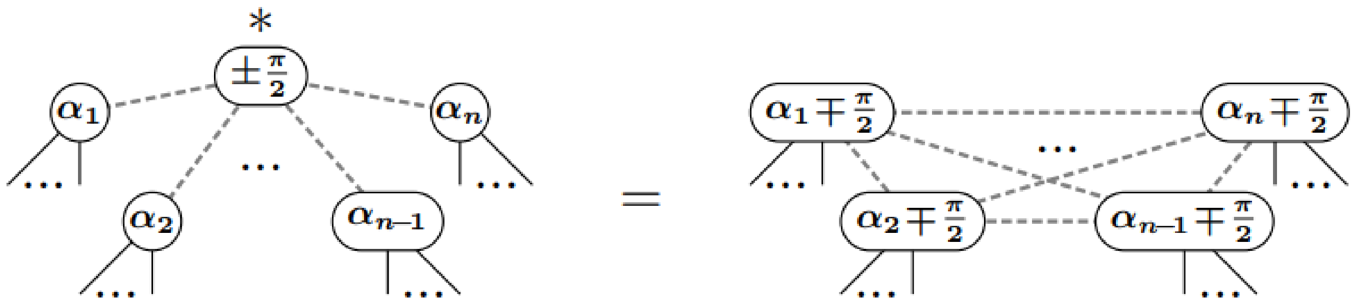
When is MB-VQE advantageous?

...translation to MB-VQE is advantageous for circuits containing a large fraction of so-called Clifford gates (e.g. CX gates), as these are absorbed into the custom state.

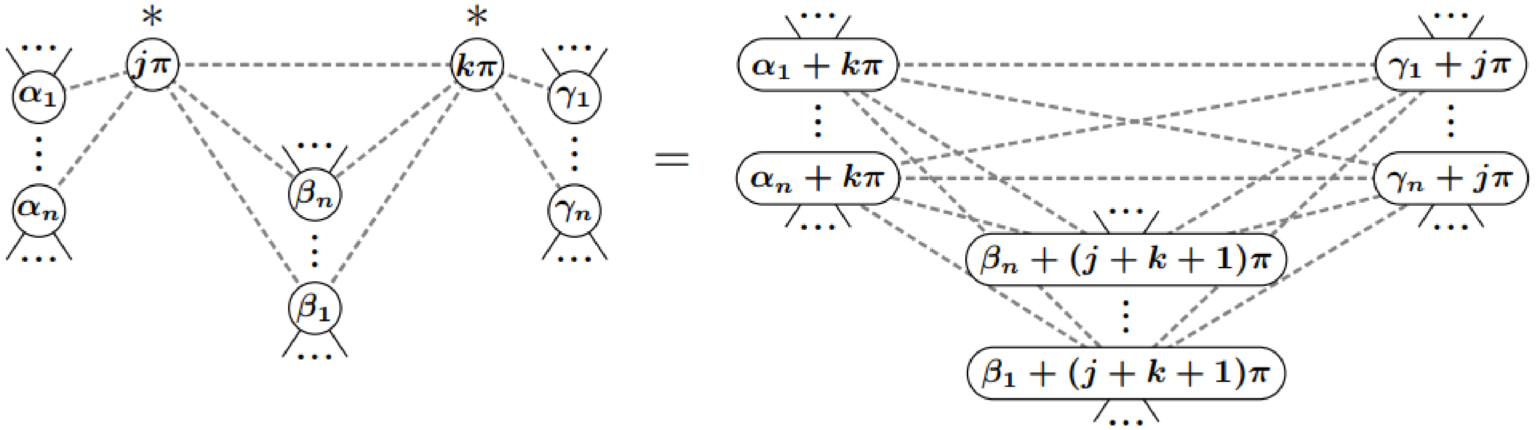
An advantage of MBQC is the possibility to simultaneously perform all non-adaptive measurements at the beginning of the calculation (...). This corresponds to the Clifford part of a circuit and includes single- and many-qubit gates. This is independent of the position of the gates in the circuit, and reduces the required overhead and coherence time. Remarkably, this can be done (...) on a classical computer before the experiment. (...) [The simplified] state can be directly prepared and used for the MBQC, which may have dramatically fewer auxiliary qubits compared to the initial graph state.

(Ferguson et al., 2021)

Simplifying the Clifford Part of Graph-Like ZX-Diagrams



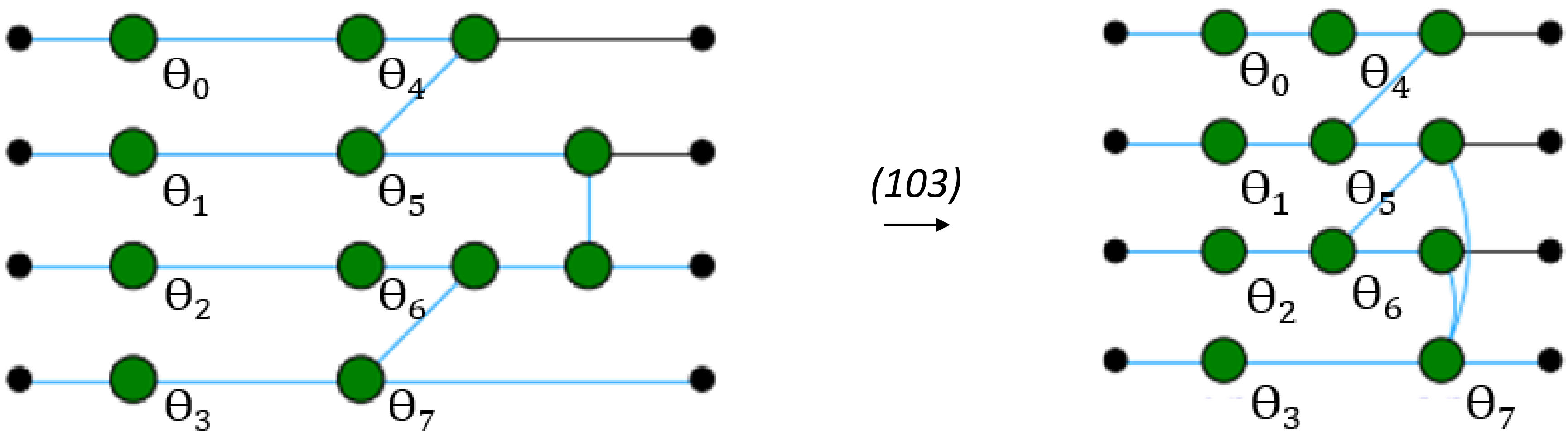
(102)



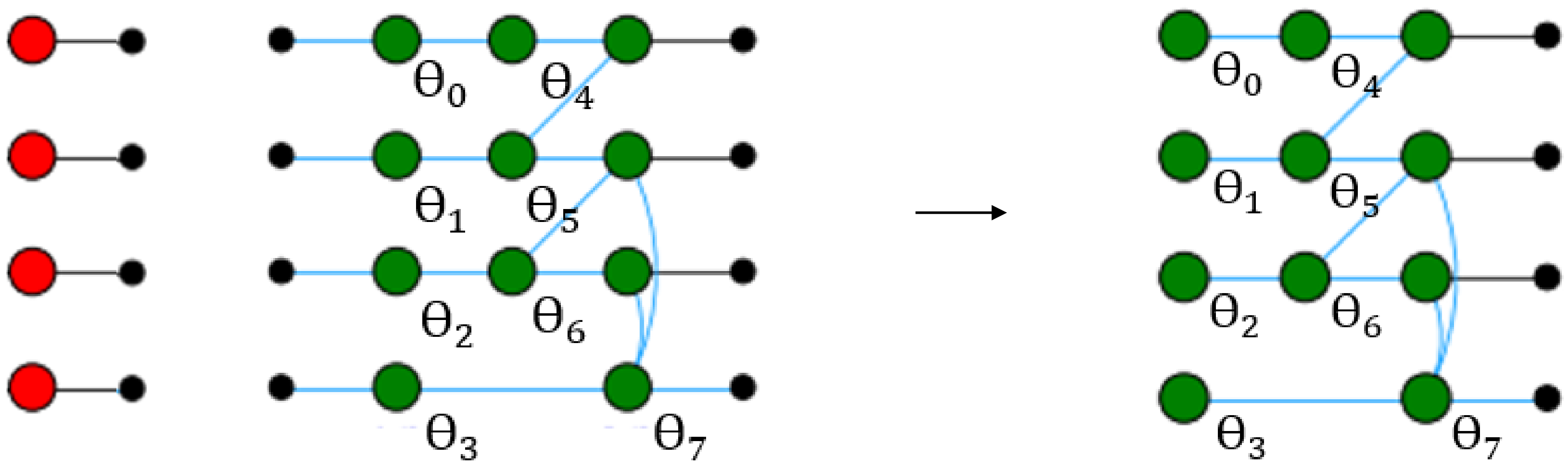
(103)

Using (102), (103), we can remove internal Clifford spiders (spiders with a phase of $k\frac{\pi}{2}, k \in \mathbb{Z}$) from the ZX diagram. That leaves only non-Clifford spiders, and border spiders.

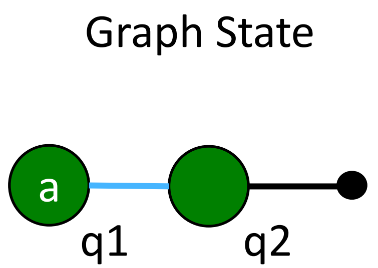
Removing Clifford Spiders from Graph-Like ZX-Diagrams

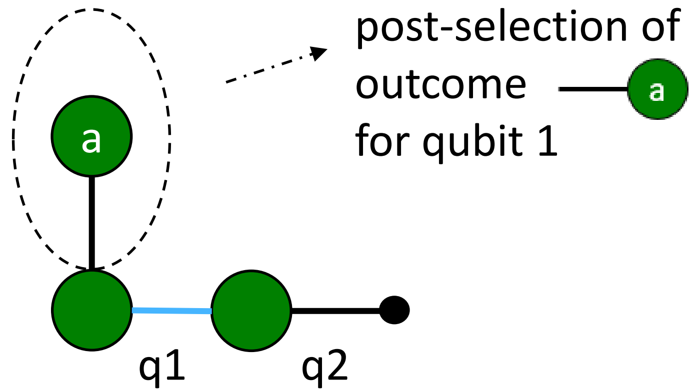


Graph States and ZX-Diagrams



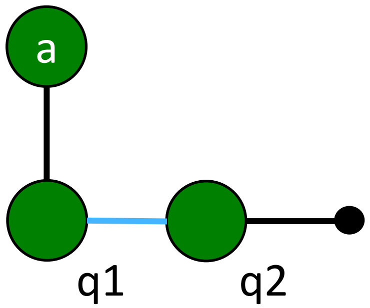
From Graph-Like ZX-Diagrams to Measurement Protocols



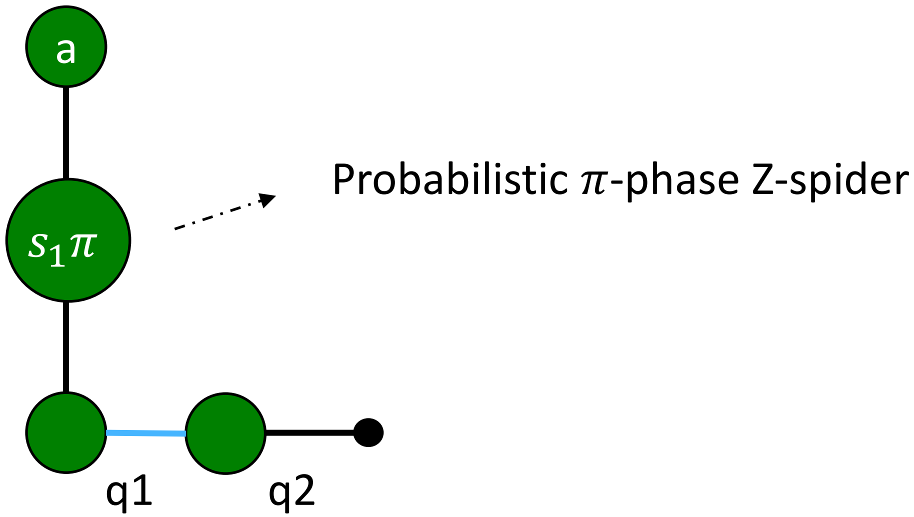


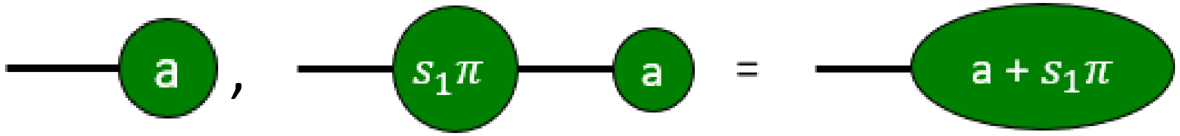
From Graph-Like ZX-Diagrams to Measurement Protocols

With post-selection



Without post-selection

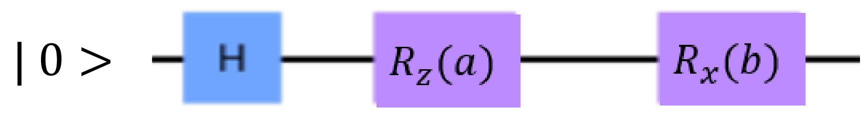


We measure qubit 1 in the basis spanned by 

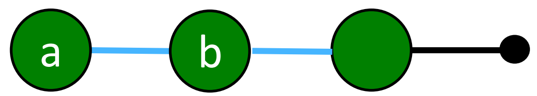
Upon measurement, we get one of these states; the probability of getting the desired one depends on the state of the qubit being measured.

From Graph-Like ZX-Diagrams to Measurement Protocols

Circuit

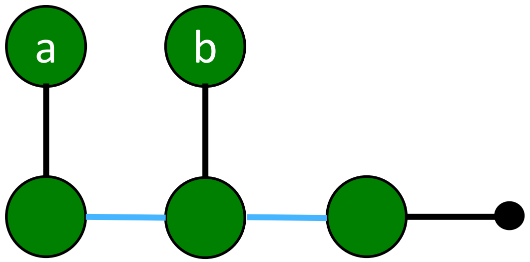


Graph-like ZX-diagram



From Graph-Like ZX-Diagrams to Measurement Protocols

With post-selection



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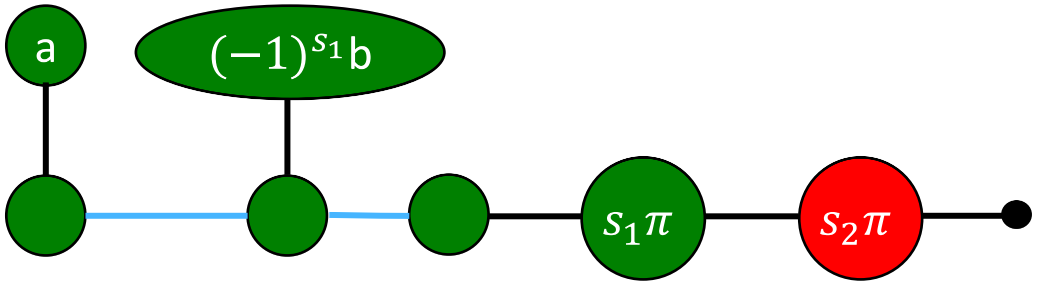
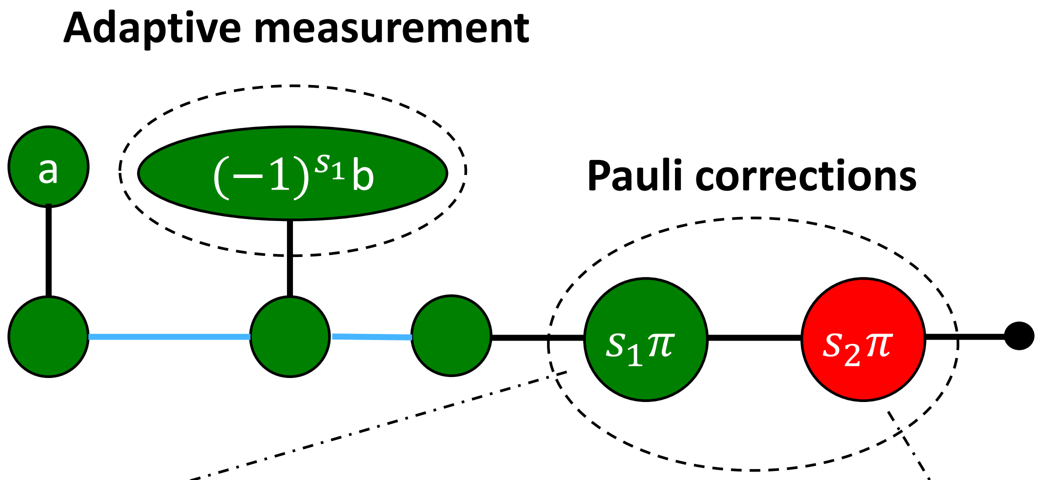


From Graph-Like ZX-Diagrams to Measurement Protocols



Pauli **Z**

We can disregard this if measuring on the computational basis (but careful with non-diagonal measurements!)

Pauli **X**

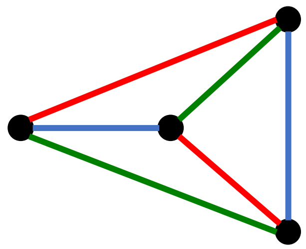
We can reinterpret measurement outcomes depending on s_2

- $\underline{s_2 = 0}$: do nothing
- $\underline{s_2 = 1}$: 0⟷1

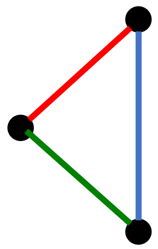
Graph State Preparation

Vizing's Theorem

A graph state on N qubits can be prepared with O(Δ) circuit depth, where Δ is the maximum degree of the graph



Class I
Depth Δ

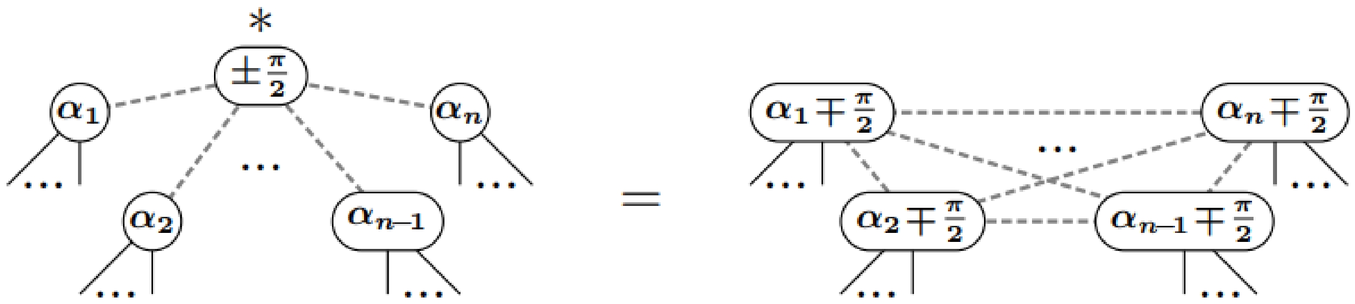


Class I
Depth Δ+1

Peter Høyer, Mehdi Mhalla, Simon Perdrix. Resources Required for Preparing Graph States. 17th International Symposium on Algorithms and Computation (ISAAC 2006), Dec 2006, Kolkata, India. pp.638 - 649, ff10.1007/11940128_64ff. ffhal-01378771f

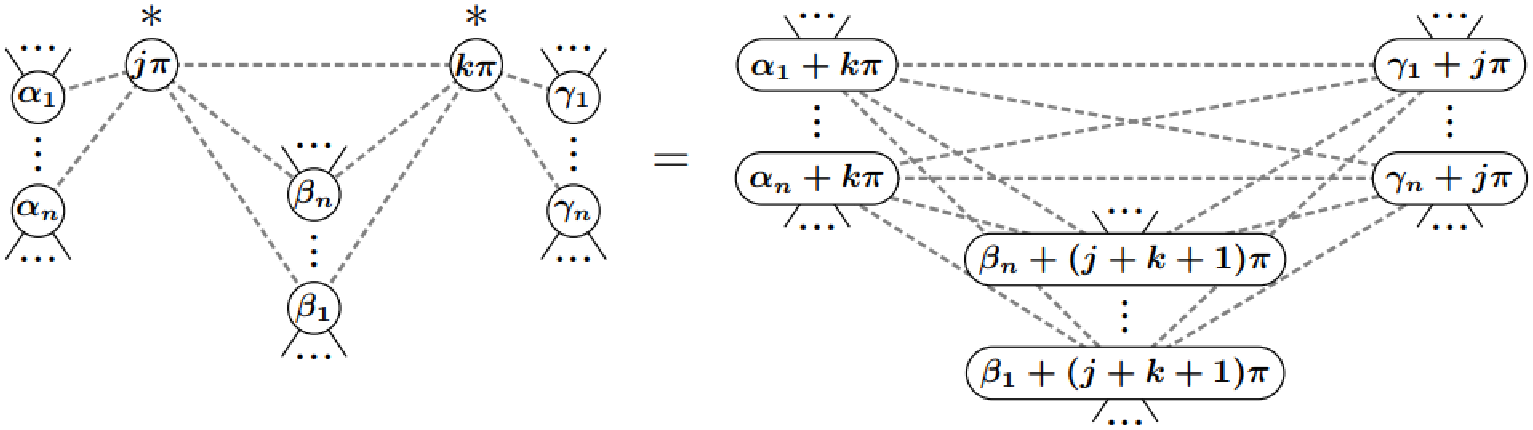
Sources of the Entangling Operations Overhead

Clifford Removal



(102)

x+4 edges *x+8 edges*



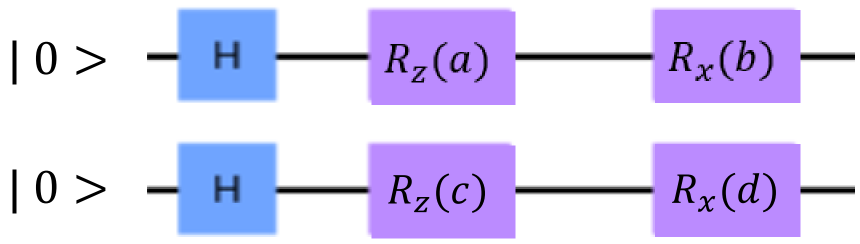
(103)

x+9 edges *x+14 edges*

Sources of the Entangling Operations Overhead

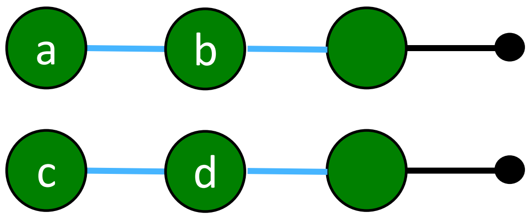
Knobs

Circuit



0 entangling operations

Graph-like ZX-diagram



4 entangling operations

Are Cliffords really 'free'?

*...translation to MB-VQE is advantageous for circuits containing a large fraction of so-called Clifford gates (e.g. CX gates), as **these are absorbed into the custom state**.*

!

Increase in graph state edge count will lead to more entangling operations and computational layers in the graph state preparation

!

*An advantage of MBQC is the possibility to simultaneously **perform all non-adaptive measurements at the beginning of the calculation** (...). This corresponds to the Clifford part of a circuit and includes single- and many-qubit gates. This is independent of the position of the gates in the circuit, and **reduces the required overhead** and **coherence time**. Remarkably, this can be done (...) on a classical computer before the experiment. (...) [The simplified] state can be directly prepared and used for the MBQC, which may have dramatically fewer auxiliary qubits compared to the initial graph state.*

! !

Entangling operation overhead can even increase

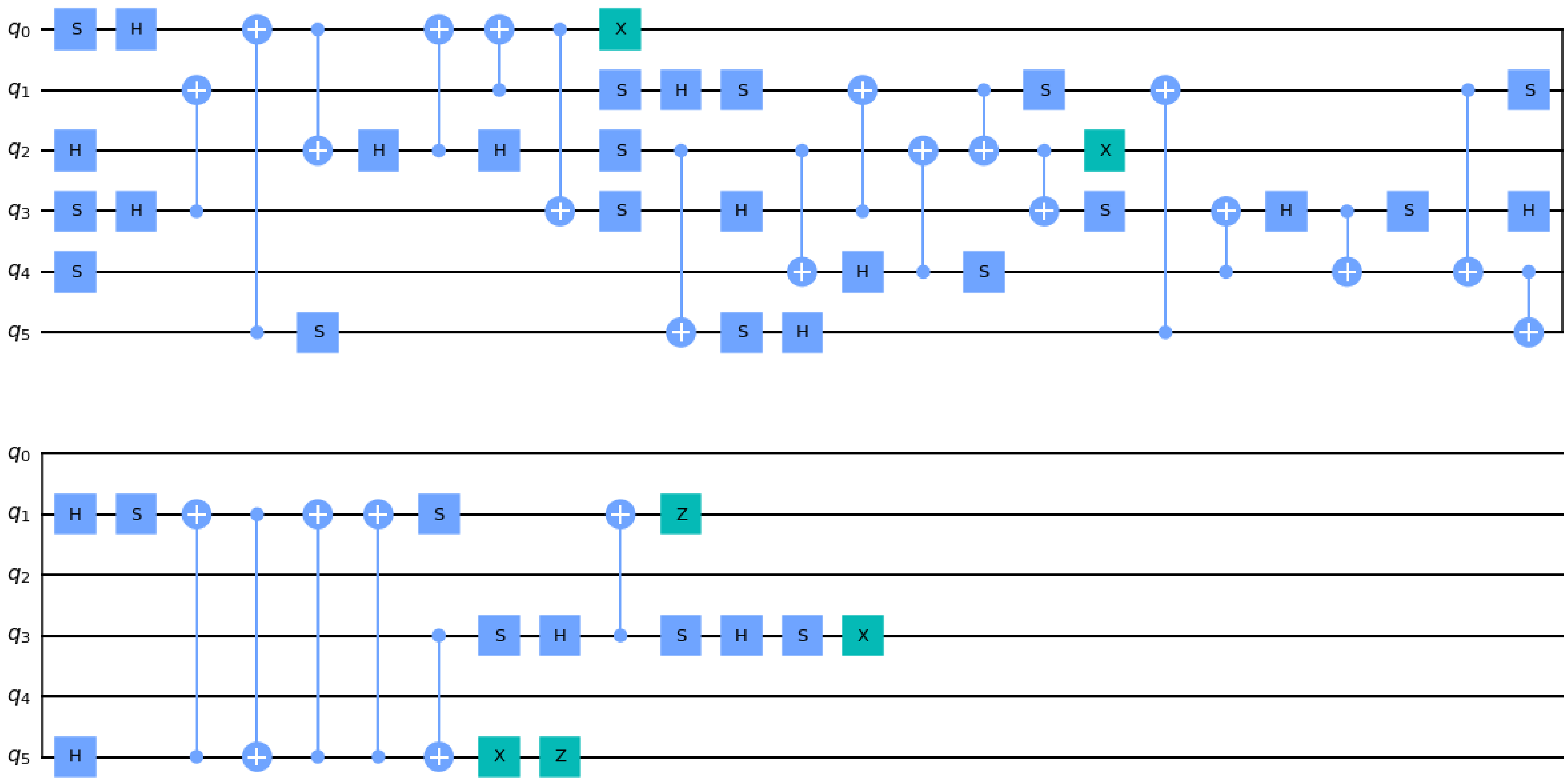
Coherence time requirements are not necessarily reduced, just shifted in part to the preparation of the resource state

... But shifting all the entangling operations into the graph state preparation allows for repeating the (probabilistic) state preparation until we know that we have the correct initial state. Cliffords are 'free' not in the sense of computational cost, but in the sense that they can in principle be exempt from errors.

(Ferguson et al., 2021)

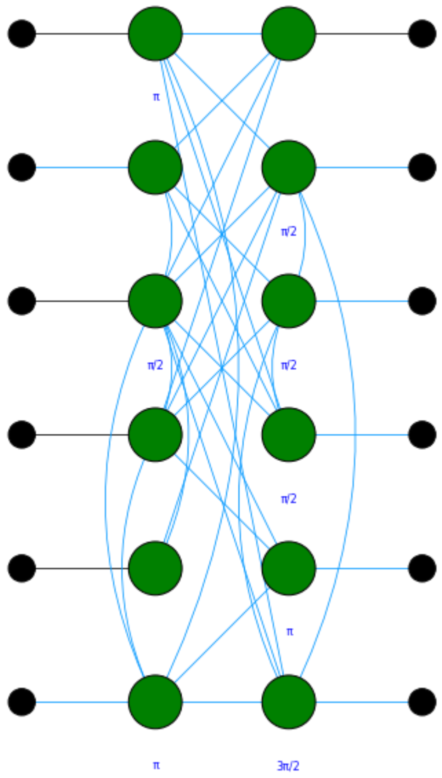
Example Global Clifford Unitary

Circuit



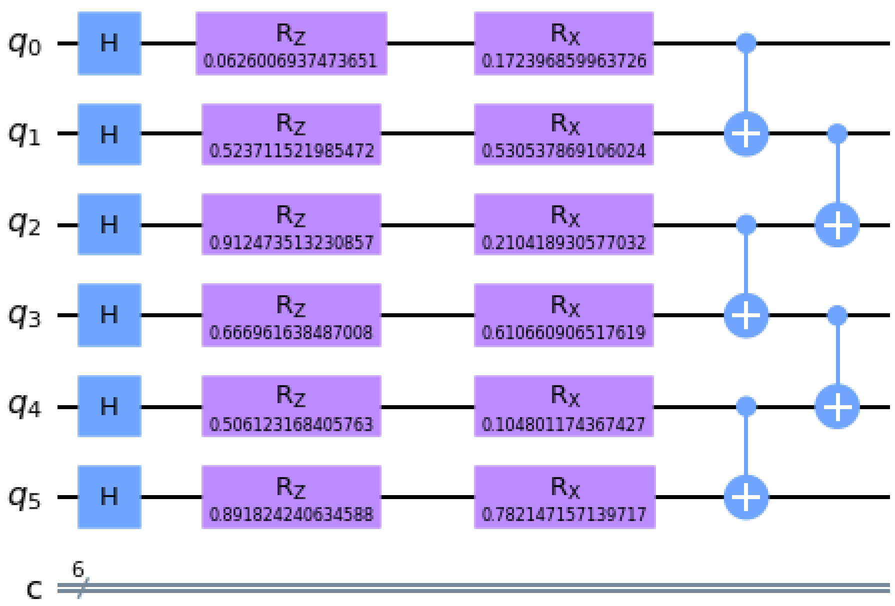
Example Global Clifford Unitary

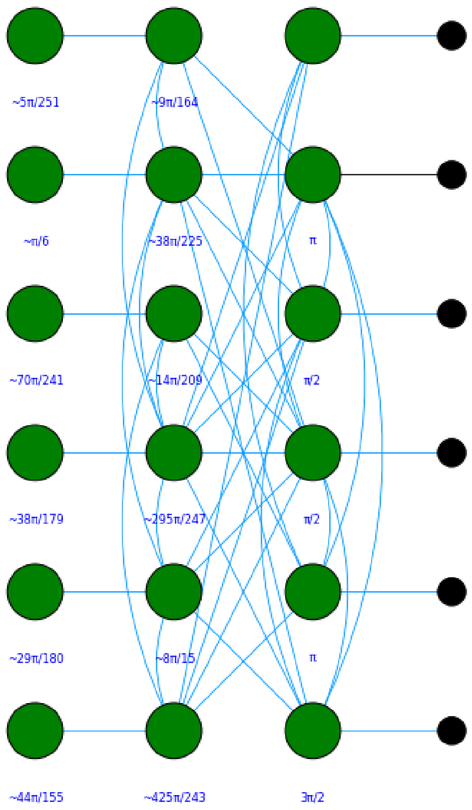
Graph-like ZX-diagram



Example State Preparation I: Hardware-Efficient Ansatz

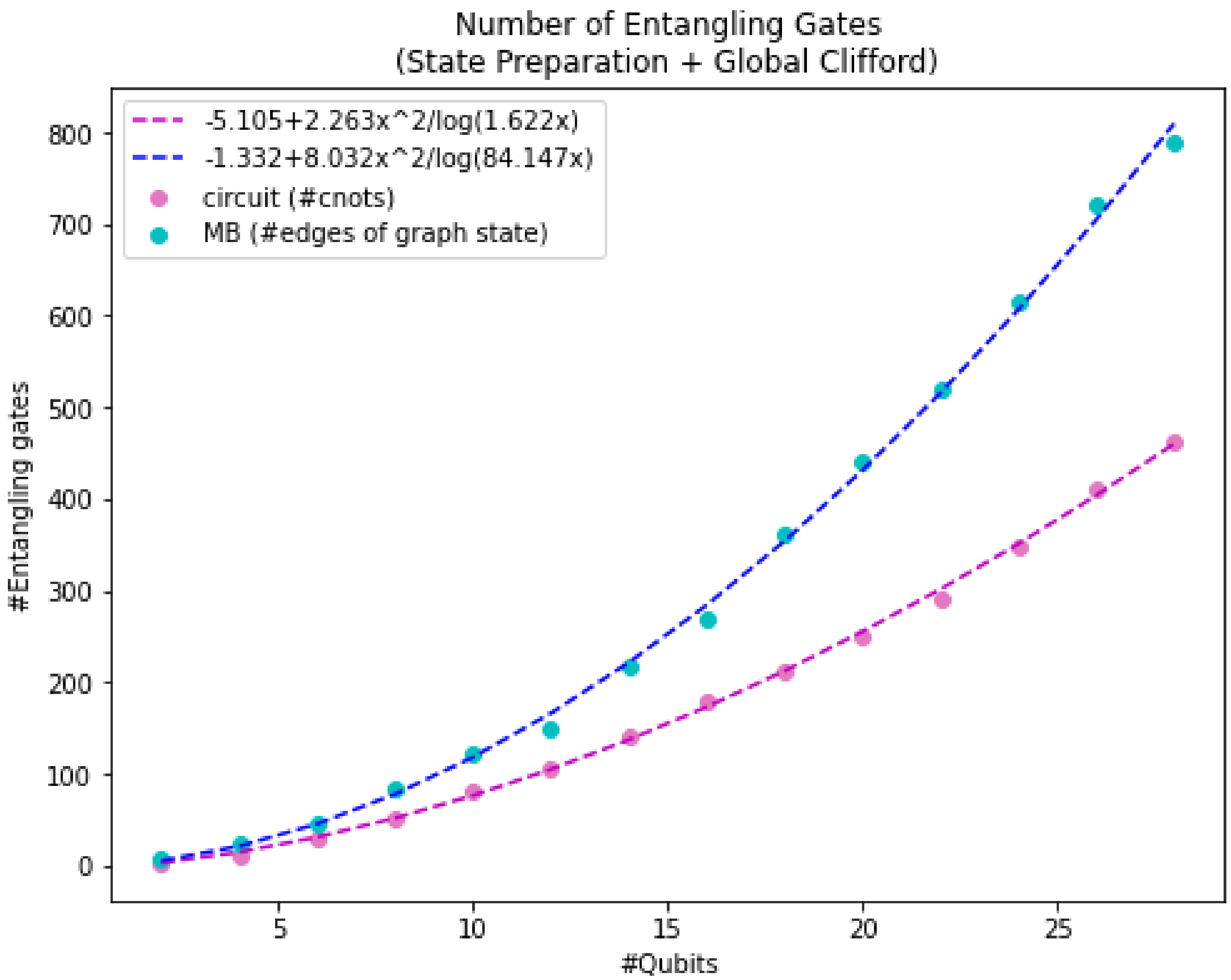
Circuit vs Graph-like ZX-diagram





Entangling Operation Count, case I (HE ansatz)

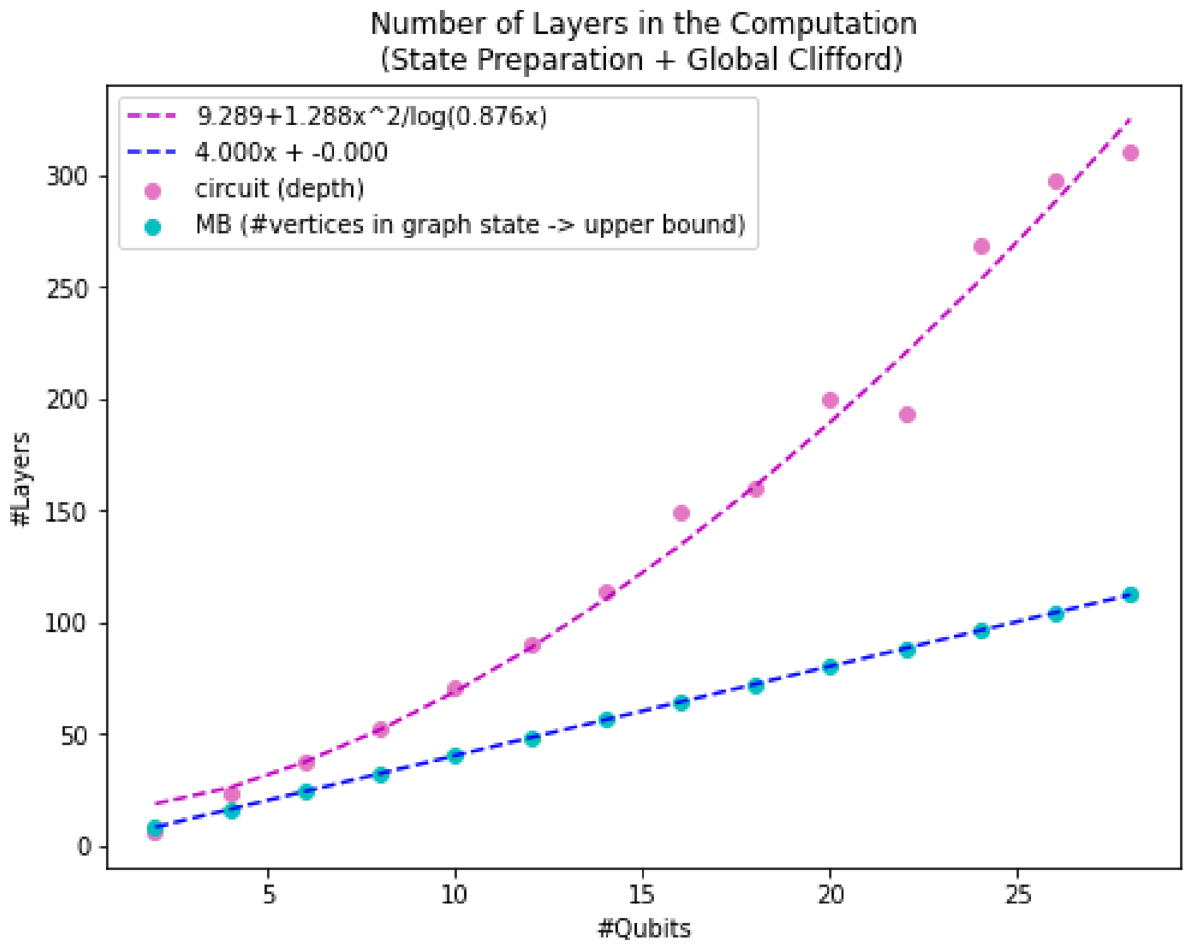
CM-VQE vs MB-VQE



- Both grow like $\mathcal{O}\left(\frac{N^2}{\log(N)}\right)$
- Better prefactor for CM-VQE
- Best choice will be platform-dependent

Number of Layers in the Computation, case I (HE ansatz)

CM-VQE vs MB-VQE



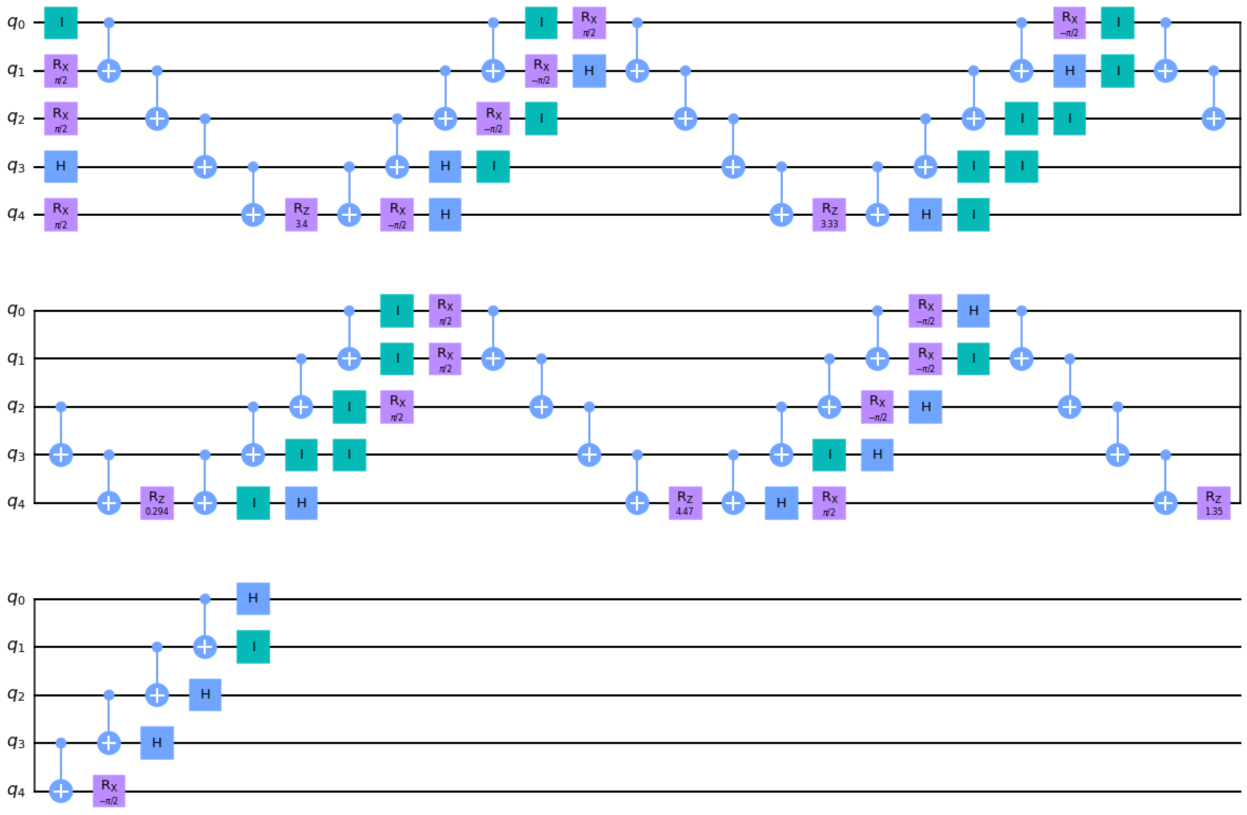
- Unoptimized CM-VQE has an associated $\mathcal{O}\left(\frac{N^2}{\log(N)}\right)$ depth
- MB-VQE has an associated $\mathcal{O}(N)$ depth from the moment the graph state is created
- Graph state creation is also $\mathcal{O}(N)$

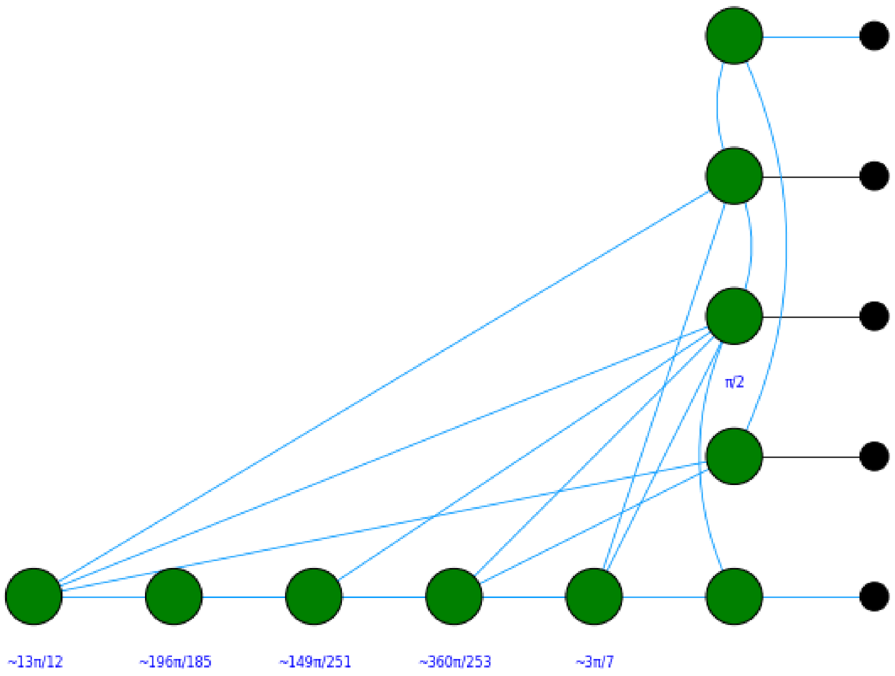
Optimized CM-VQE (LNN)*: $\sim 9n$
Full MB-VQE: $\sim 5n$

*Bravyi et al., 2021

Example State Preparation II: N Pauli Exponentials

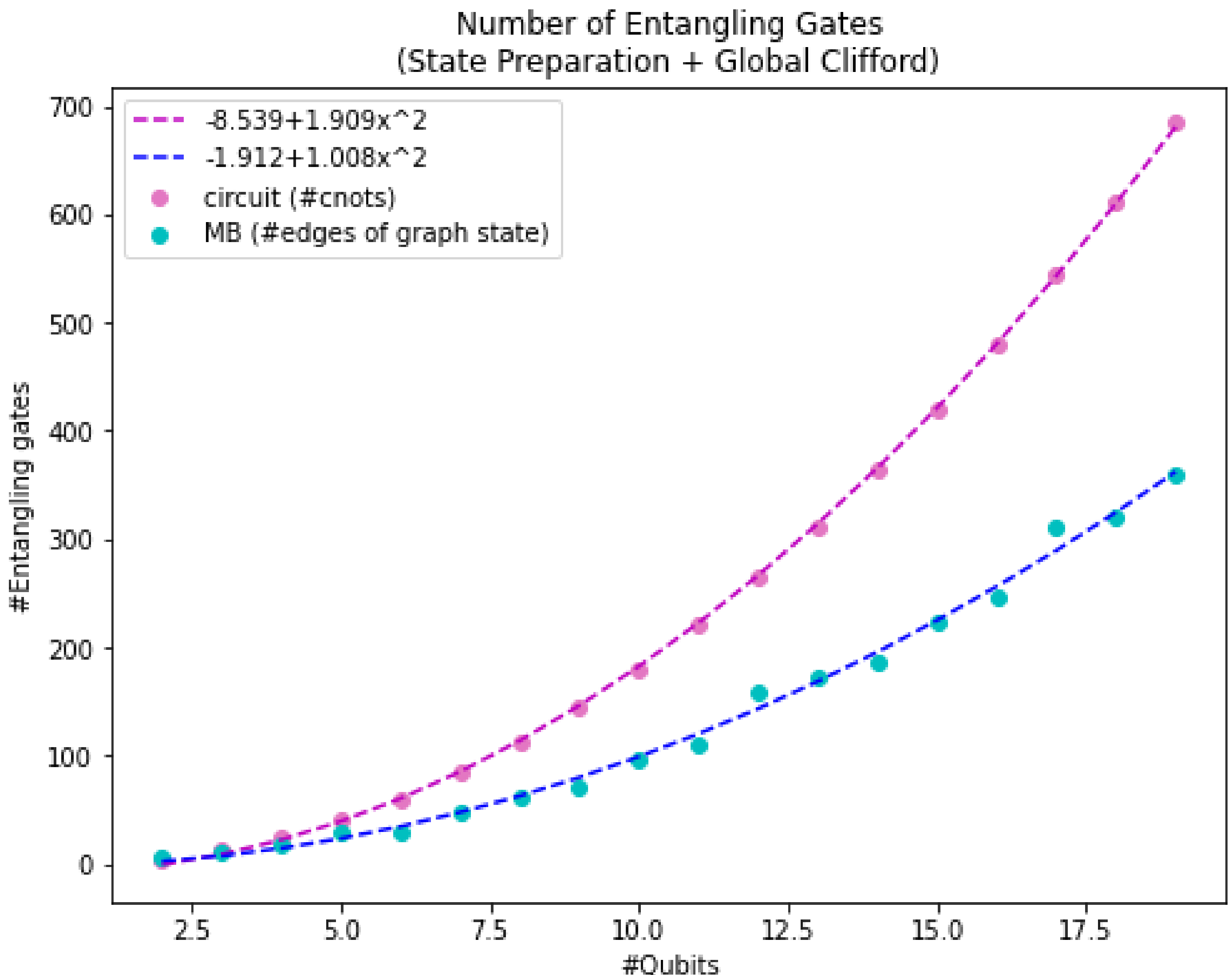
Circuit vs Graph-like ZX-diagram





Entangling Operation Count, case II (*N* PE Ansatz)

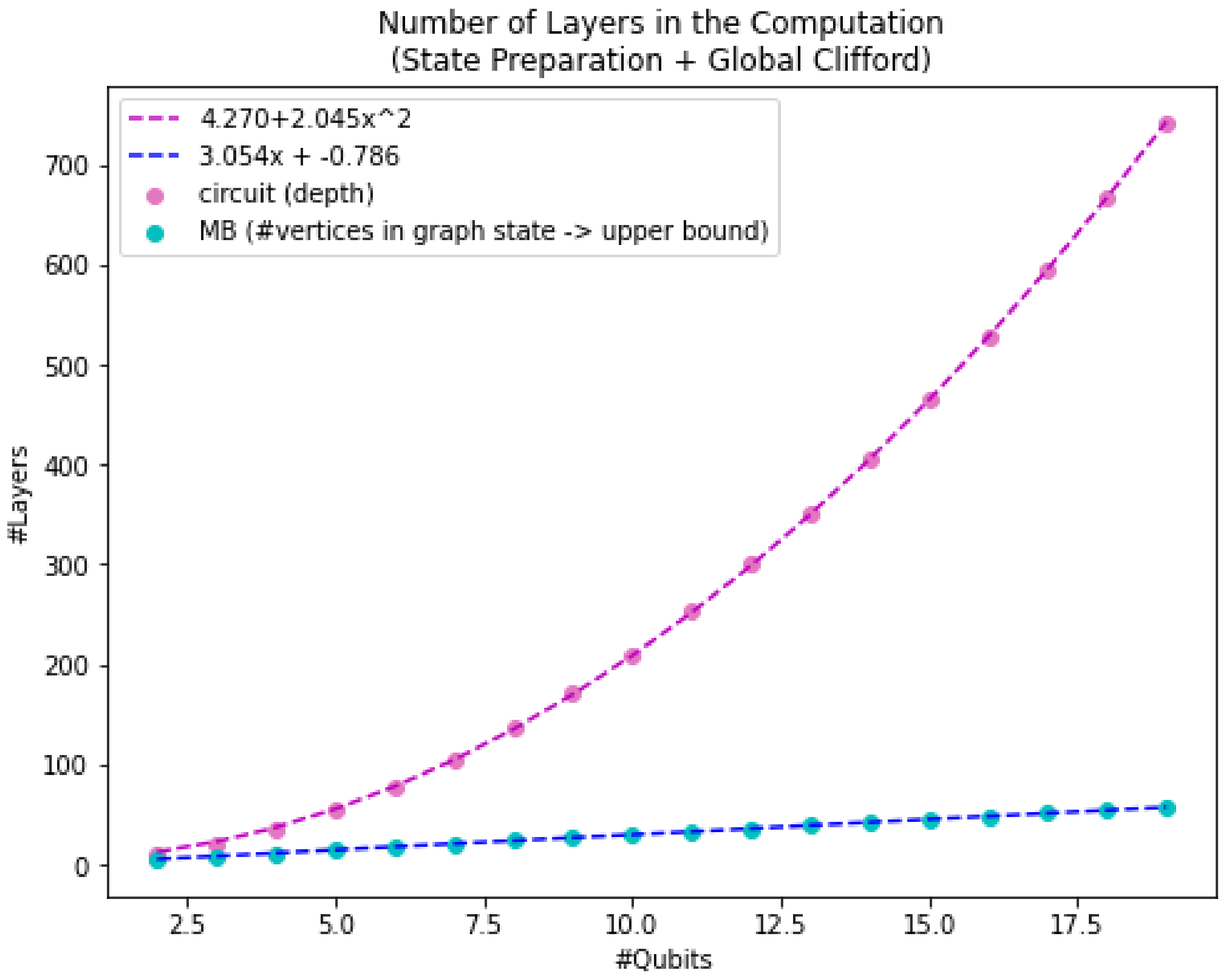
CM-VQE vs MB-VQE



- Both grow like $\mathcal{O}\left(\frac{N^2}{\log(N)}\right)$
- Better prefactor for MB-VQE
- Best choice will be platform-dependent

Number of Layers in the Computation, case II (*N* PE Ansatz)

CM-VQE vs MB-VQE



- Unoptimized CM-VQE has an associated $\mathcal{O}\left(\frac{N^2}{\log(N)}\right)$ depth
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- Graph state creation is also $\mathcal{O}(N)$

Optimized CM-VQE (LNN): $\sim 9n$
Full MB-VQE: $\sim 4n$

Classical Shadows

Theorem 1 (informal version). *Classical shadows of size N suffice to predict M* arbitrary *linear target functions* $\mathrm{tr}(O_1\rho), \ldots, \mathrm{tr}(O_M\rho)$ *up to additive error ϵ given that $N \geq$ (order)* $\log(M) \max_i \|O_i\|^2_{\mathrm{shadow}} / \epsilon^2$. *The definition of the norm $\|O_i\|_{\mathrm{shadow}}$ depends on the ensemble of unitary transformations used to create the classical shadow.*

Scenario: observables with a bounded Hilbert-Schmidt norm $Tr(O^2)$

- Applying global random Cliffords at the end of the circuit (along with some classical processing steps) allows for an exponential decrease in the number of samples required for estimating the expectation values of M observables
- With $\mathcal{O}(\log(M))$ shots we can estimate the value of M observables; with $\mathcal{O}(M)$ of e^M
- Number of shots is independent of the size of the system

(Huang et al., 2020)

Classical Shadows

(global Cliffords)

Extra cost (circuit model)

$\mathcal{O}\left(\frac{N^2}{\log(N)}\right)$ entangling operations

$\mathcal{O}(N)$ depth

Extra cost (MBQC)

$\mathcal{O}\left(\frac{N^2}{\log(N)}\right)$ entangling operations

$\mathcal{O}(N)$ depth

Applications

- Quantum fidelity estimation (QFE)
- Entanglement verification (via entanglement witnesses)

Classical Shadows

(global Cliffords)

Classical shadows and MB-VQE

- Shot requirements are currently a major limitation of VQAs
- MB-VQE could offer a better prefactor for the depth (especially if the ansatz also has a large Clifford part)
- Channeling the difficulty towards the preparation of an entangled resource state can benefit certain platforms

Issue: it's rare for variational algorithms to target observables with a bounded Hilbert-Schmidt norm

Fermionic Classical Shadows

Theorem 1.—Consider all $2k$-degree Majorana operators $\Gamma_{\boldsymbol{\mu}}$ on n fermionic modes, labeled by $\boldsymbol{\mu} \in \mathcal{C}_{2n,2k}$. Under the ensemble $\mathcal{U}_{\mathrm{FGU}}$ defined in Eq. (11), the shadow norm satisfies

$$\|\Gamma_{\boldsymbol{\mu}}\|^2_{\mathrm{FGU}} = \binom{2n}{2k} \Big/ \binom{n}{k} \approx \binom{n}{k}\sqrt{\pi k} \qquad (15)$$

for all $\boldsymbol{\mu} \in \mathcal{C}_{2n,2k}$. Thus the method of classical shadows estimates the fermionic k-RDM of any state ρ, i.e., $\mathrm{tr}(\Gamma_{\boldsymbol{\mu}}\rho)\ \forall\ \boldsymbol{\mu} \in \cup_{j=1}^{k} \mathcal{C}_{2n,2j}$, to additive error ε, given

$$M = \mathcal{O}\left[\binom{n}{k}\frac{k^{3/2}\log n}{\varepsilon^2}\right] \qquad (16)$$

copies of ρ.

- The fermionic version of classical shadows allows for an improvement in the number of samples required to evaluate the k-RDM of a quantum state
- Calculating the k-RDM allows us to determine the expectation value of any k-body observable
- The strategy is tailored to local fermionic observables, which do **not** correspond to local qubit observables

(Zhao et al., 2021)

Hamiltonian averaging

Variance of estimator (Ha)

Molecule (qubits)	CS (Pauli)	CS (FGU)
H_2 (8)	51.4	69.6
LiH (12)	266	155
BeH_2 (14)	1670	586
H_2O (14)	2840	8440
NH_3 (16)	14400	5846
	(Huang et al., 2020)	(Zhao et al., 2021)

Fermionic classical shadows allow for an improvement over the random Pauli classical shadows...

Hamiltonian averaging

Variance of estimator (Ha)

Molecule (qubits)	CS (Pauli)	CS (FGU)	LBCS
H_2 (8)	51.4	69.6	17.5
LiH (12)	266	155	14.8
BeH_2 (14)	1670	586	67.6
H_2O (14)	2840	8440	257
NH_3 (16)	14400	5846	353
	(Huang et al., 2020)	(Zhao et al., 2021)	(Hadfield et al., 2020)

Fermionic classical shadows allow for an improvement over the random Pauli classical shadows...

... but don't beat the state-of-the-art for Hamiltonian averaging.

Can fermionic classical shadows be tailored to the specific problem of Hamiltonian averaging to improve this result?

Can MB-VQE offer an advantadge in the search for a minimum of another fermionic k-body observable?

Conclusions

- MB-VQE shifts the main workload of VQE into the preparation of an entangled resource state, after which the computation amounts to nothing but measurements

- This new algorithm may be more suitable for e.g. photonic quantum computers

- Important costs (e.g. entangling operations) are ‘hidden’ in the resource state

- The best choice between CM- and MB-VQE is platform-dependent and trade-offs must be carefully analysed

References

MB-VQE

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MBQC

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ZX-Calculus

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- Kissinger, A., & van de Wetering, J. (2020). PyZX: Large Scale Automated Diagrammatic Reasoning. Electronic Proceedings in Theoretical Computer Science, 318, 229–241. https://doi.org/10.4204/EPTCS.318.14

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Clifford circuits

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