
JAMES
What is the ground state energy of my molecule?

LOQCathon Team 6: Shadow VQE

Team: Eduardo Beattie, Maria Gragera Garces, Shin Nishio, Lia Yeh, Hafsa Zeroual
Mentor: Benjamin Stott (Quandela)

1. Introduction
    a. The **Variational Quantum Eigensolver**
    b. Classical Shadows

2. Our implementation of shadow VQE
    a. Circuit layout
    b. Software architecture
    c. Results

3. Extensions
    a. Execution on the cloud QPU
    b. 4-qubit system
    c. Cluster states for VQE

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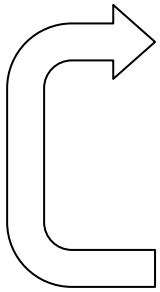
The Variational Quantum Eigensolver

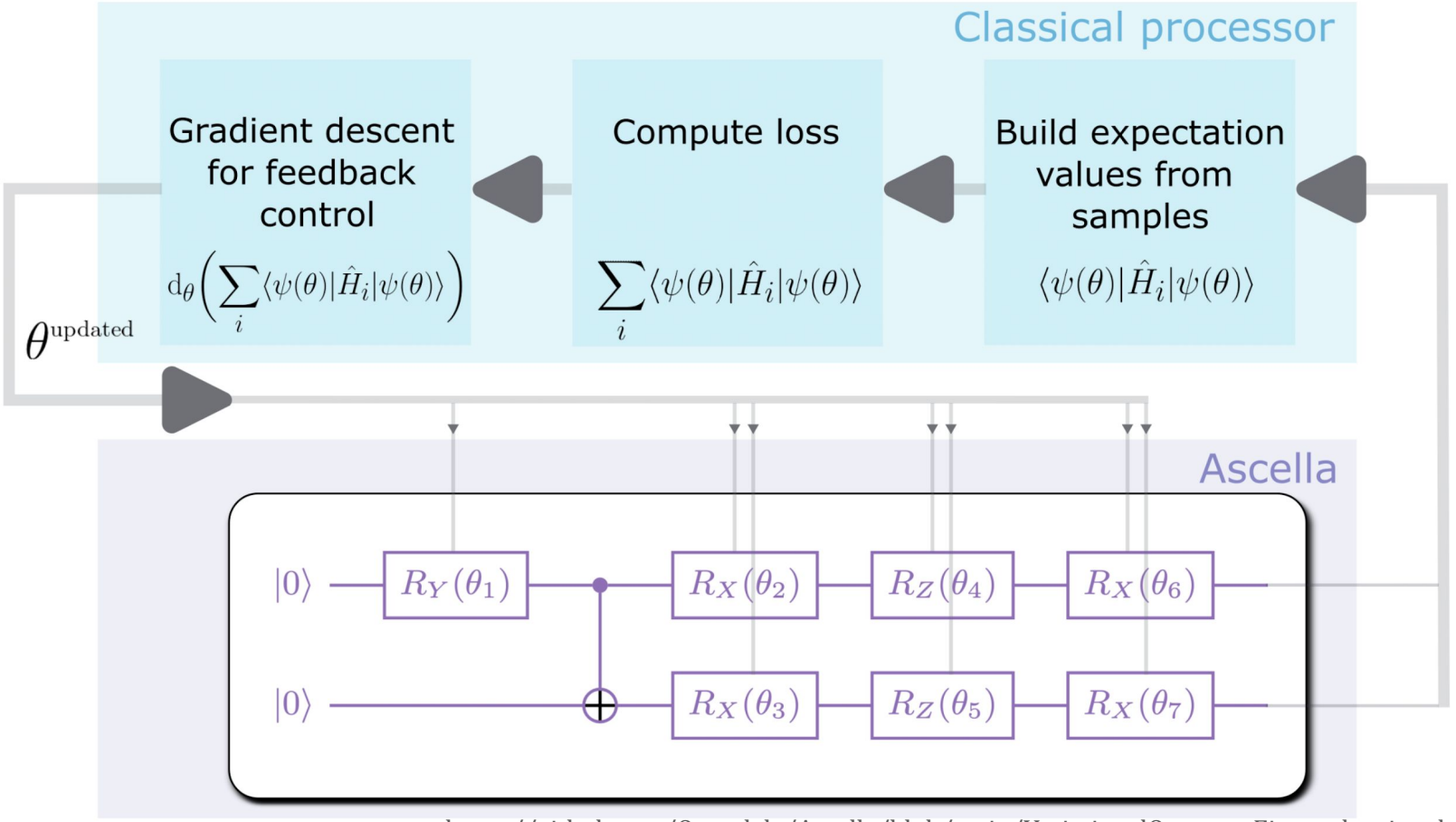
GOAL: Find the ground state of a given Hamiltonian

1. Prepare a guess of the solution (ansatz)
2. Measure the expectations of every Pauli string
3. Classically evaluate the Hamiltonian

4. update



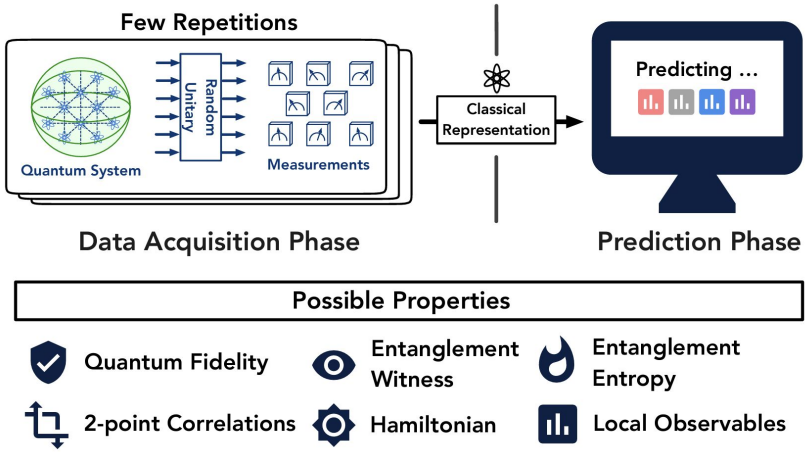
The Variational Quantum Eigensolver



https://github.com/Quandela/Ascella/blob/main/VariationalQuantumEigensolver.ipynb

Classical Shadow

"...an efficient method for constructing an **approximate classical description** of a quantum state using very few measurements"



Huang, Hsin-Yuan, Richard Kueng, and John Preskill.
"Predicting many properties of a quantum system from very few measurements."
Nature Physics 16.10 (2020): 1050-1057.
doi: 10.1038/s41567-020-0932-7

Tomography

Pick **all unitary U** from a Clifford group
Where Clifford group is defined as

$$C_n = \{U \in U_{2^n} | UP_iU^\dagger = P_j\}$$

Which has $2^{n^2}\prod_{j=1}^{n}(2^{2j}-1)$ elements

e.g. n=6
2.1×10^{23}

Then we can construct the table

$$\begin{bmatrix} \rho_{1,1} & \rho_{1,2} & \cdots & \rho_{1,n} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{m,1} & \rho_{m,2} & \cdots & \rho_{m,n} \end{bmatrix}$$

Classical Shadow

Pick unitaries Us **randomly** from a tomographically complete set (e.g. Pauli group, Clifford group)

$$\rho \rightarrow U\rho U^\dagger$$

We get "snapshot"

$$\mathbb{E}[U^\dagger |b\rangle \langle b| U] = \mathcal{M}(\rho)$$

We can reconstruct the original state

$$\rho = \mathbb{E}[\mathcal{M}^{-1}U^\dagger |b\rangle \langle b| U]$$

We can also estimate any observable with the empirical mean

$$\langle O \rangle = \frac{1}{N}\sum_i Tr\hat{\rho}_i O$$

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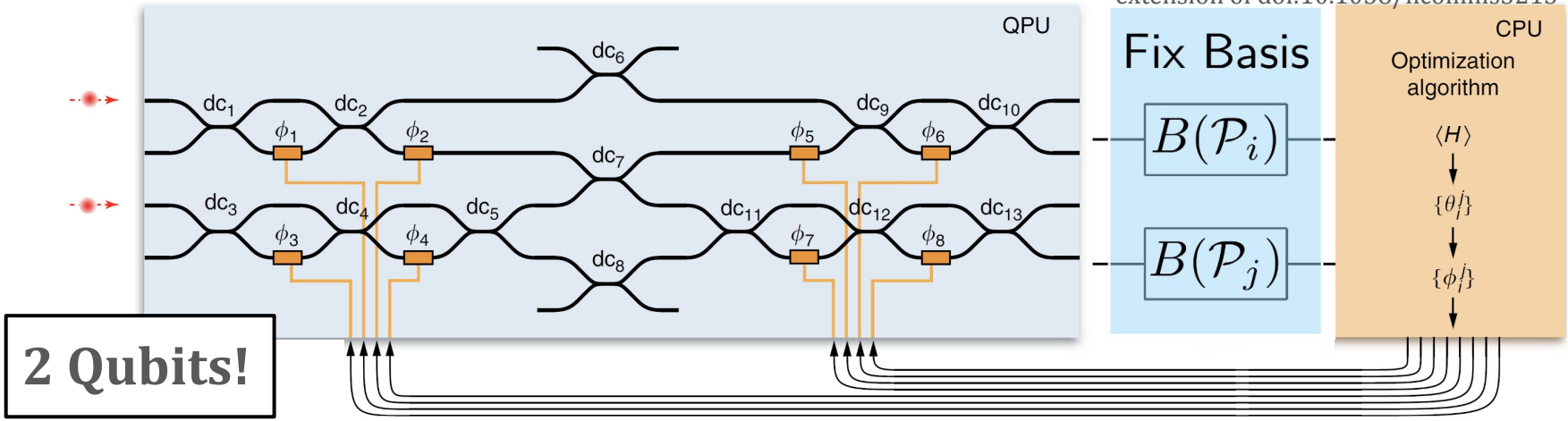
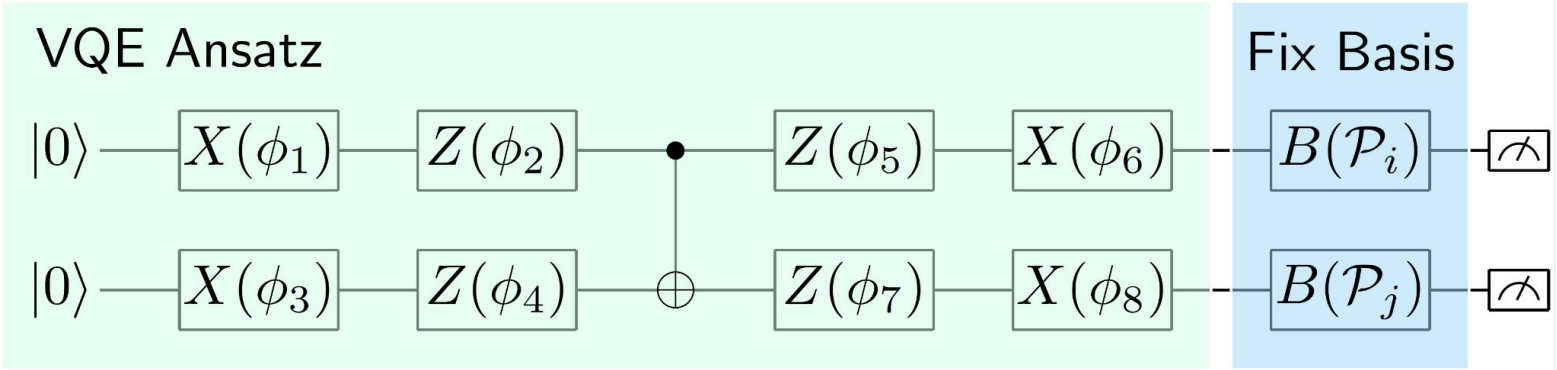
H2 Shadow-VQE optical circuit in Perceval

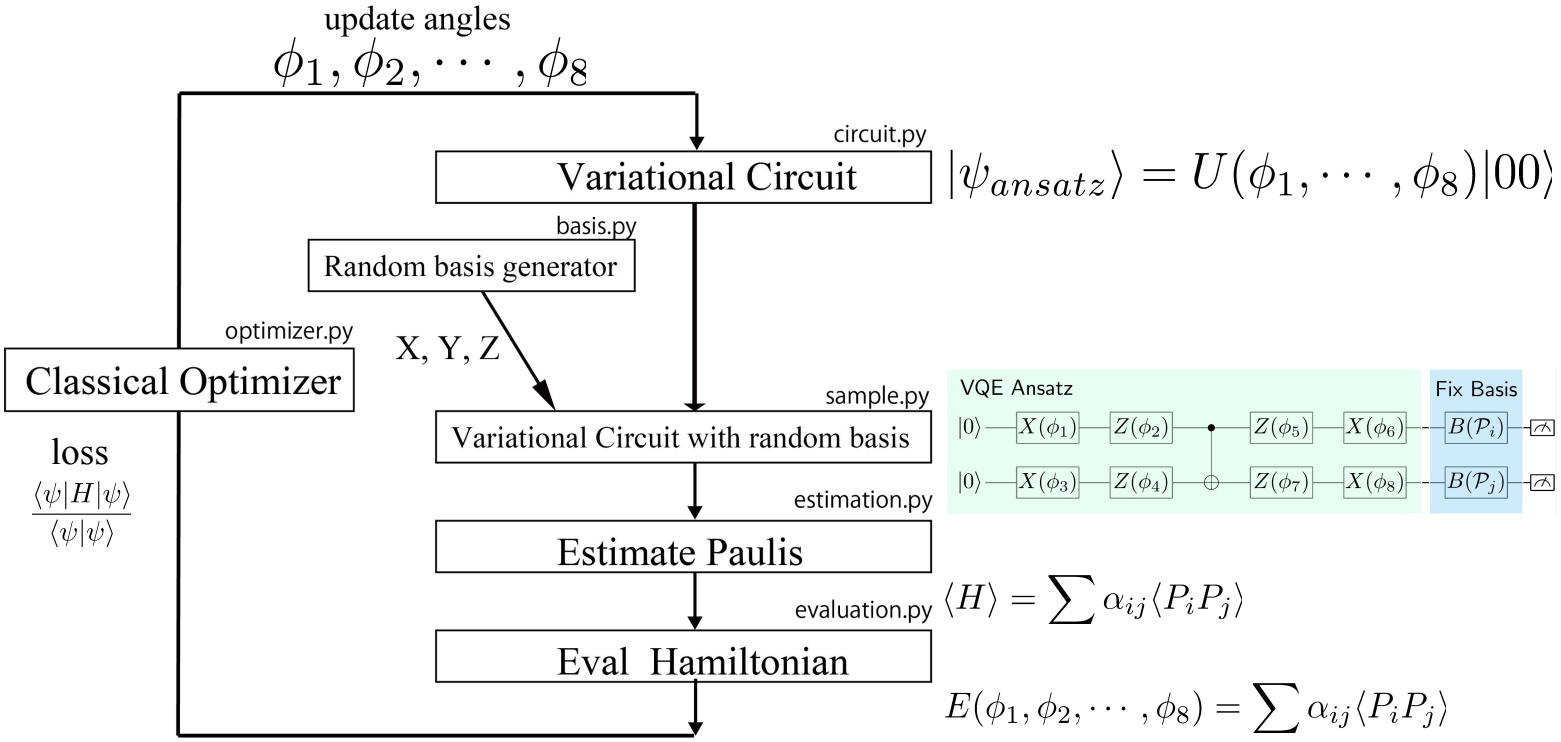
extension of doi:10.1038/ncomms5213



2 Qubits!



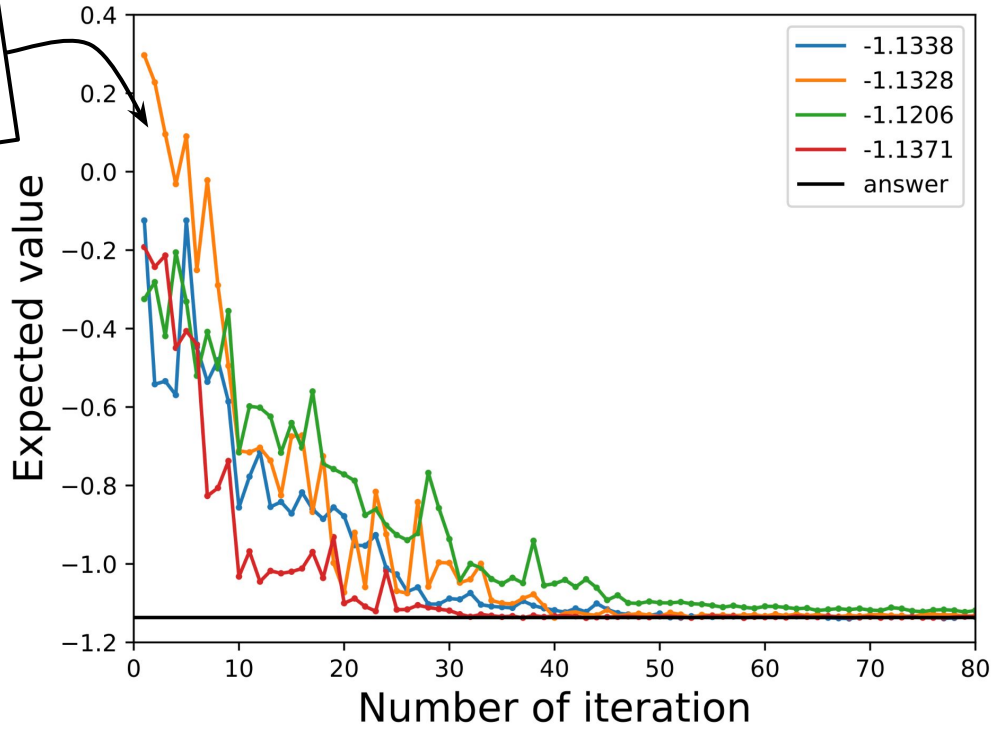
Software Architecture for Shadow-VQE

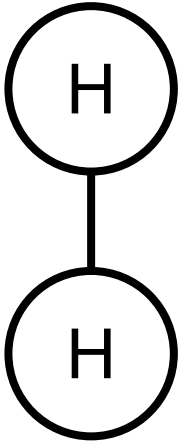


Our implementation converges on the solution!

N = 100,000, Goal = -1.1367

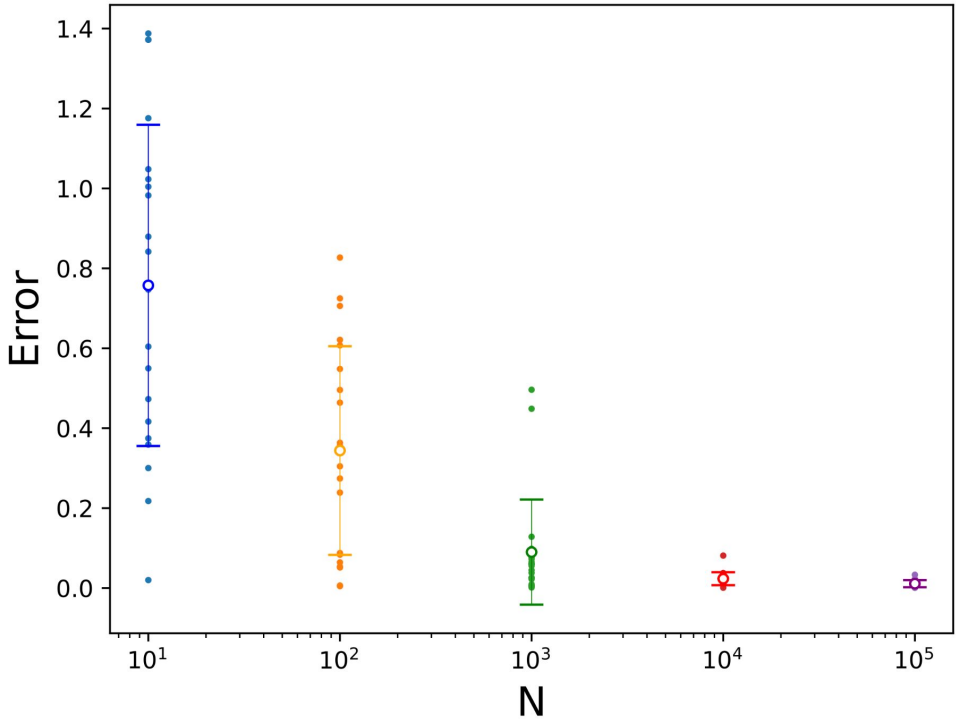
4 random initial states





Our Hamiltonian is the H2 molecule.

More measurements reduce the error.



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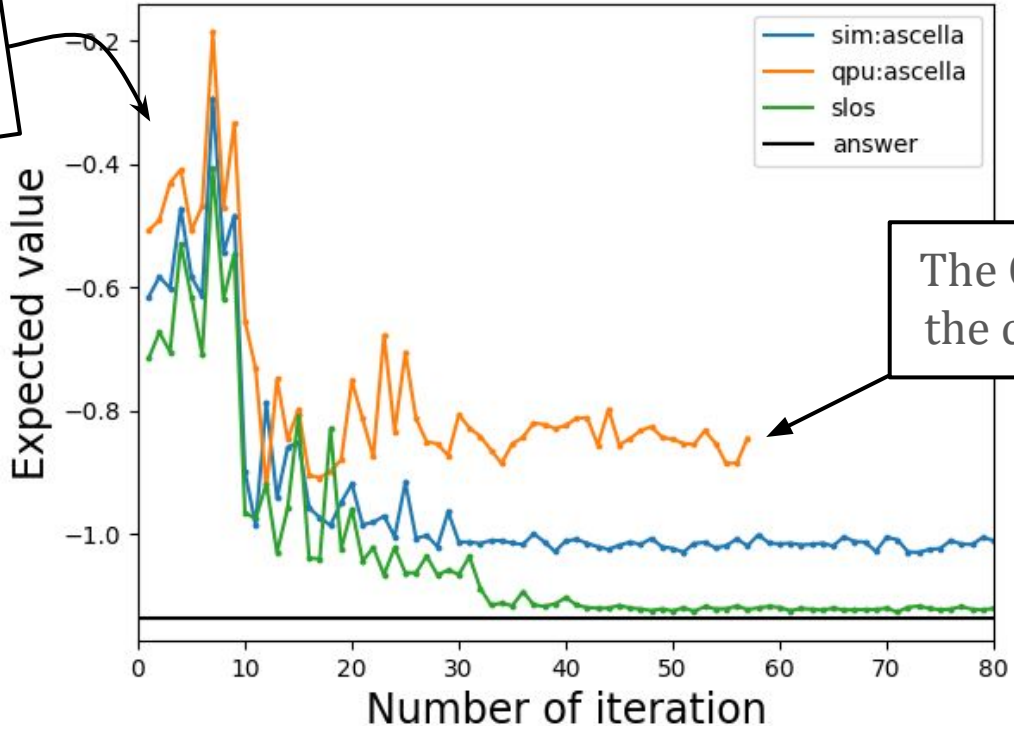
We ran the algorithm on the cloud QPU.

N = 50,000, Goal = -1.1367

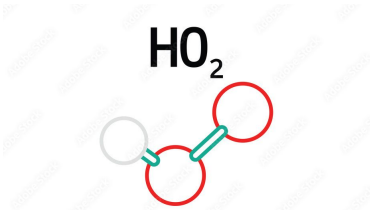
Same random initial state



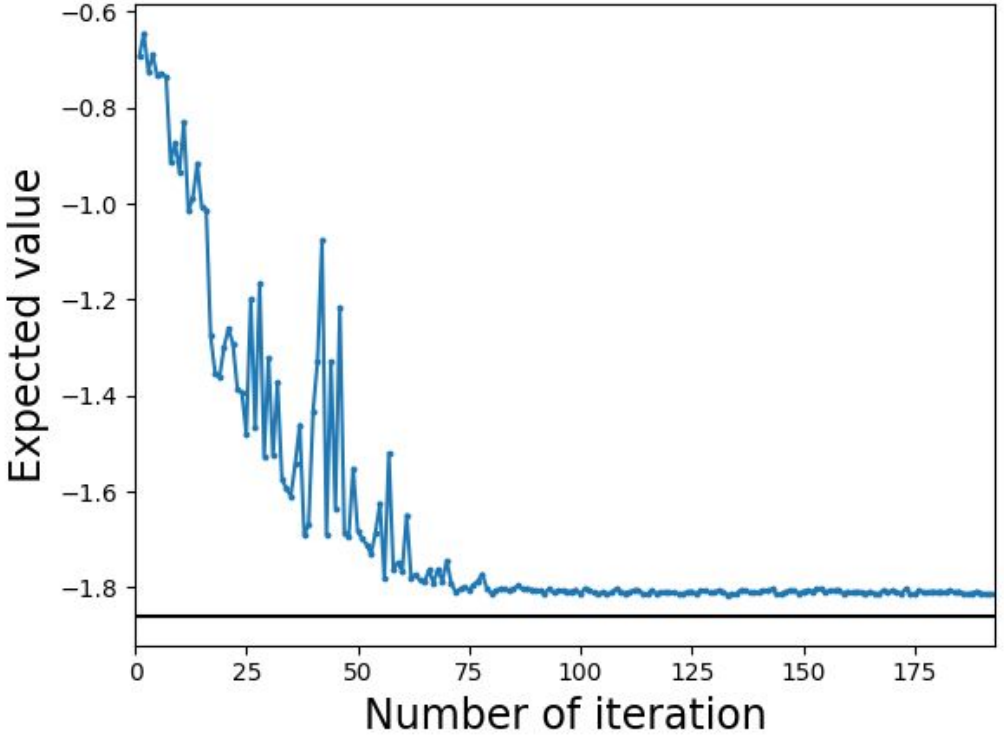
The QPU's noise affects the convergence value.

Bonus Implementation: 4 qubit infrastructure

4 qubits
12 modes

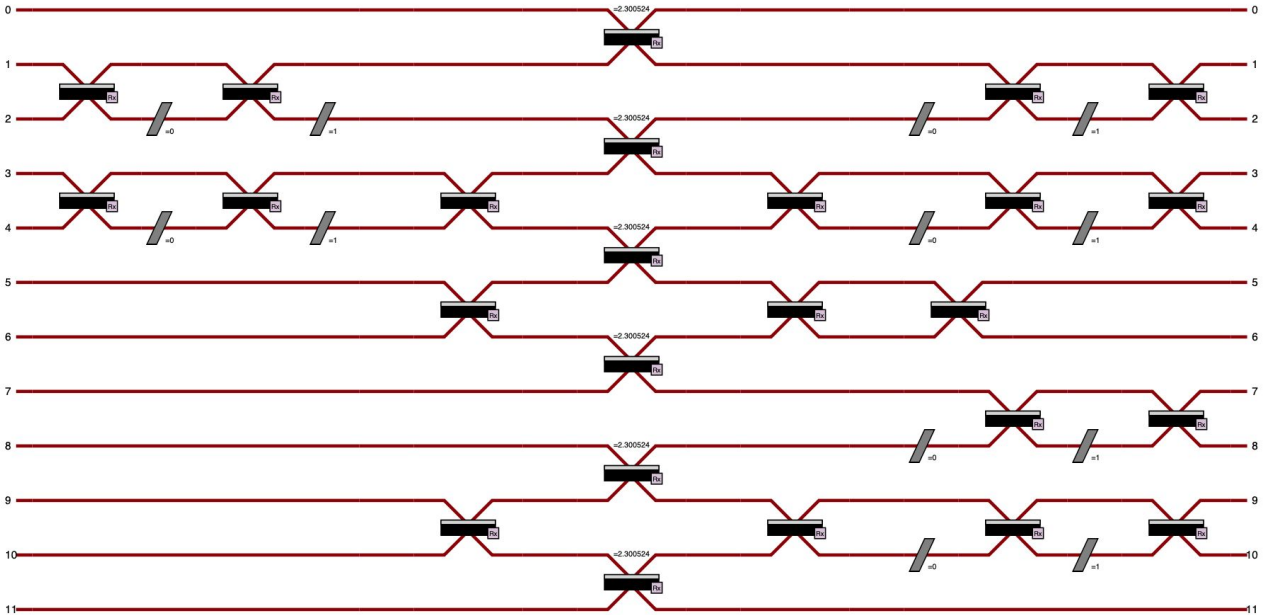


Objective = -1.86
Result = -1.81



Bonus Implementation: 4 qubit infrastructure

Next steps: implement an optimized ansatz for the problem at hand



Bonus Challenge: Cluster State Implementation

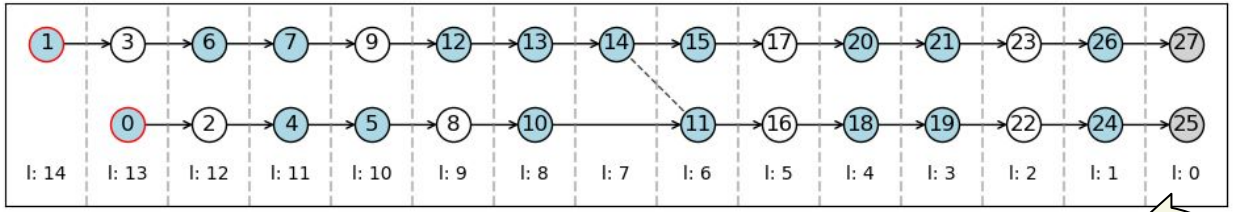
- For the bonus challenge, we were asked to improve the VQE implementation by generating entanglement from cluster states instead of gates.

- In the absence of software tailored to fusion-based quantum computation, we present our solution and proposed implementation.

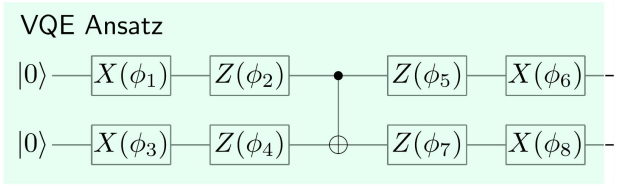
Bonus Challenge: Cluster State Implementation

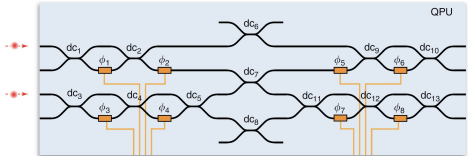
```
N, node = 1
N, node = 3
E, nodes = (1, 3)
M, node = 1, plane = XY, angle(pi) = 0
N, node = 0
N, node = 2
E, nodes = (0, 2)
M, node = 0, plane = XY, angle(pi) = 0
N, node = 6
E, nodes = (3, 6)
M, node = 3, plane = XY, angle(pi) = -1
N, node = 4
E, nodes = (2, 4)
M, node = 2, plane = XY, angle(pi) = -1
N, node = 7
E, nodes = (6, 7)
M, node = 6, plane = XY, angle(pi) = 0,
E, nodes = (4, 5)
M, node = 4, plane = XY, angle(pi) = 0
```

N: prepare |+> state
E: apply CZ between a pair of qubits
M: Measure in specific plane

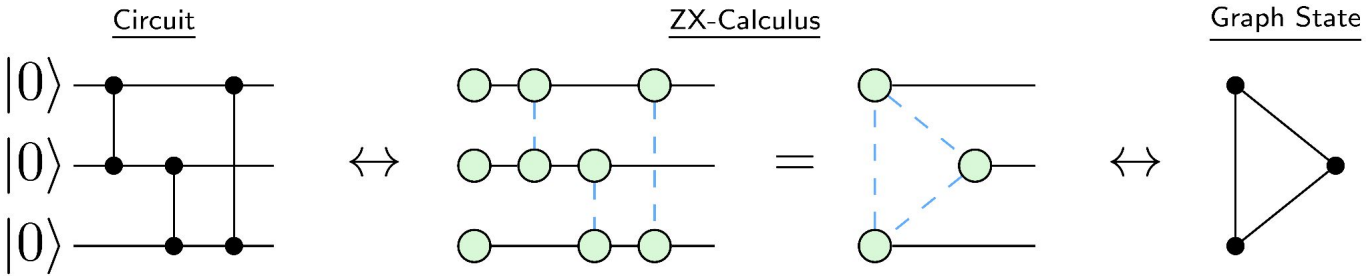


Above: Optimized implementation in Graphix MBQC library of the below circuit

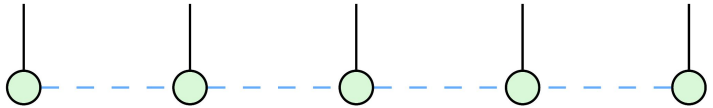




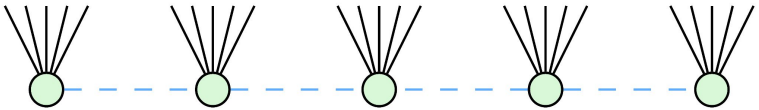
Linear Optics + Fusion Measurement + Classical Feed-forward = Universal Quantum Computation



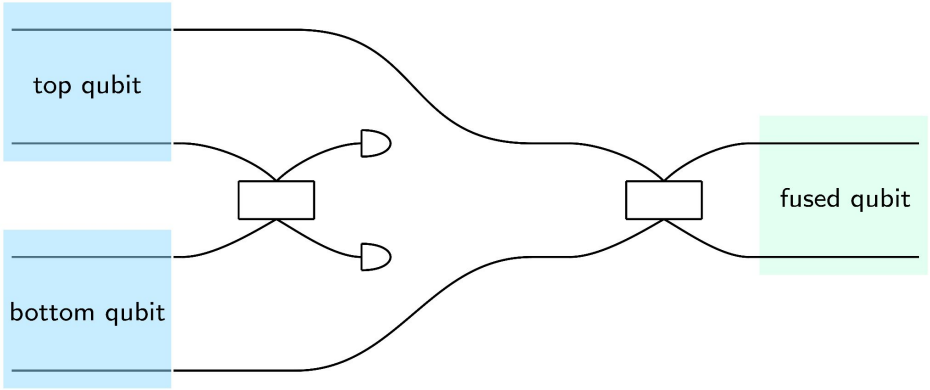
Linear Cluster State



Quandela's Generated Resource State



Dual Rail Encoding: Fusion Measurement



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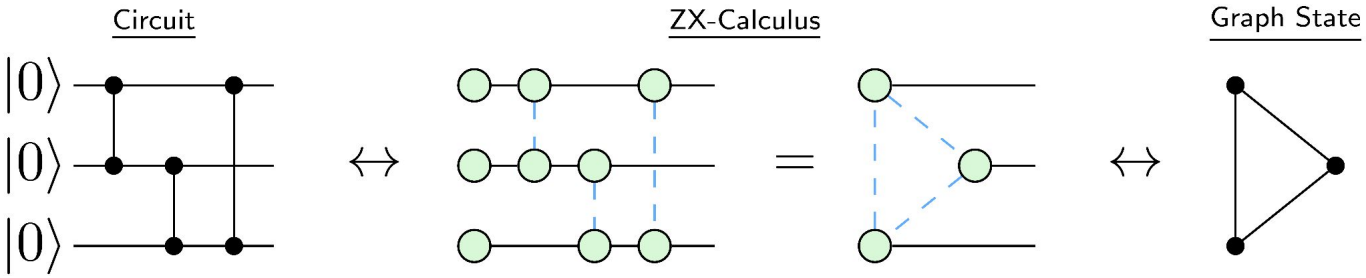
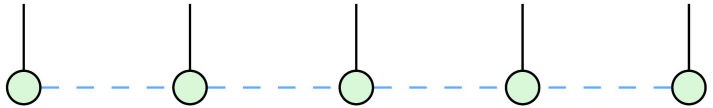
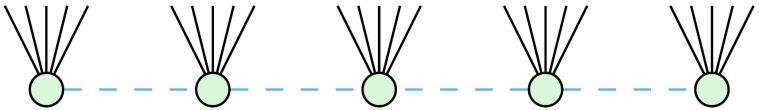


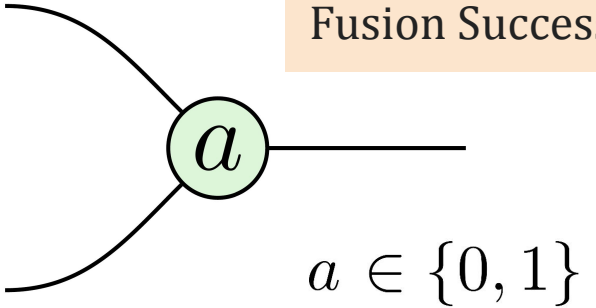
Linear Cluster State



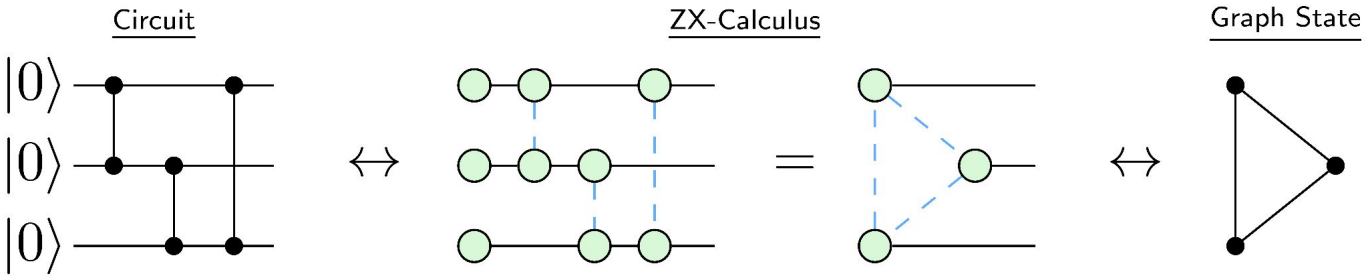
Quandela's Generated Resource State



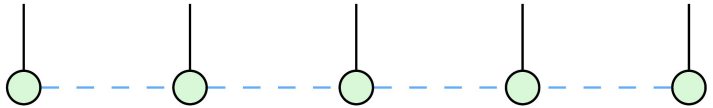
Dual Rail Encoding: Fusion Measurement



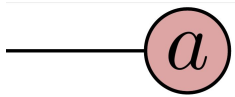
Linear Optics + Fusion Measurement + Classical Feed-forward = Universal Quantum Computation



Linear Cluster State

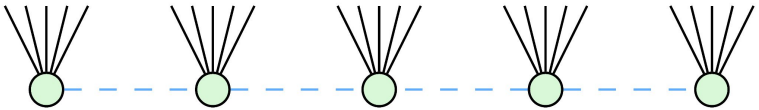


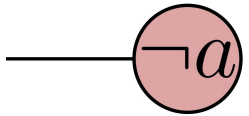
Dual Rail Encoding: Fusion Measurement



Fusion Failure

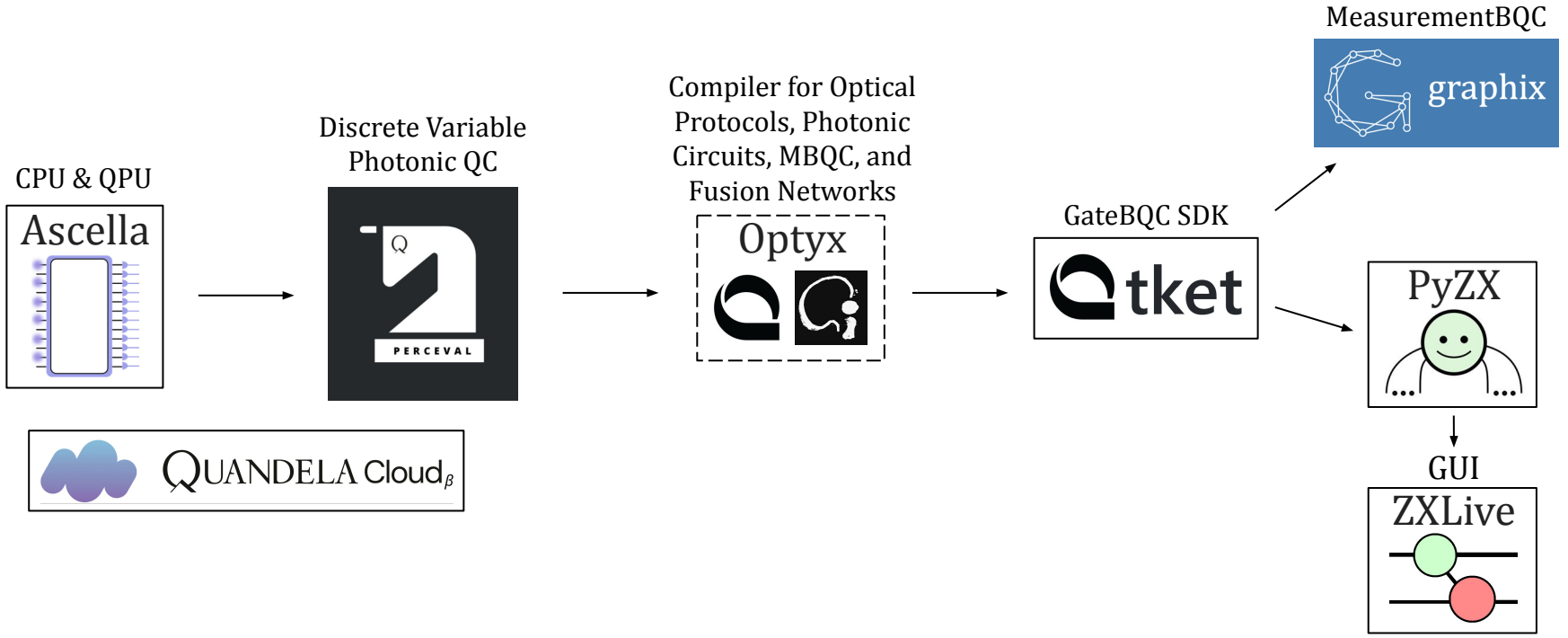
Quandela's Generated Resource State





$a \in \{0, 1\}$

Software Pipeline for Cluster-Shadow-VQE



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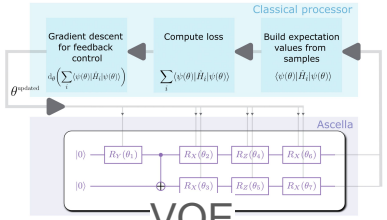
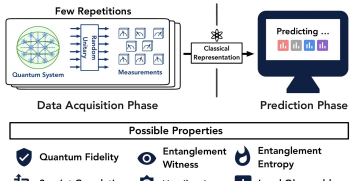
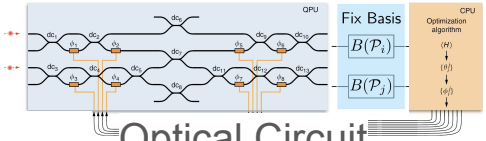


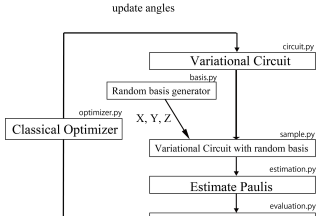
VQE



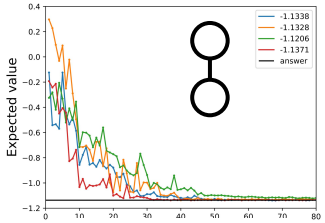
Classical Shadows



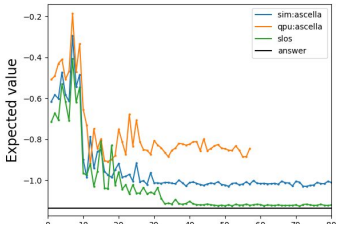
Optical Circuit



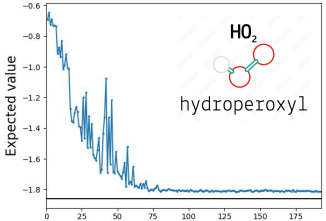
Software Architecture



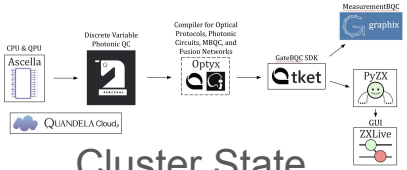
Convergence



Cloud QPU Execution



4 qubits



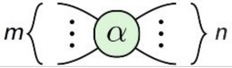
Cluster State Software Pipeline

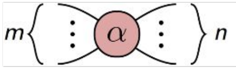
Supplementary slides

ZX-Calculus: prove any equality of qubit linear maps in just 8 rules

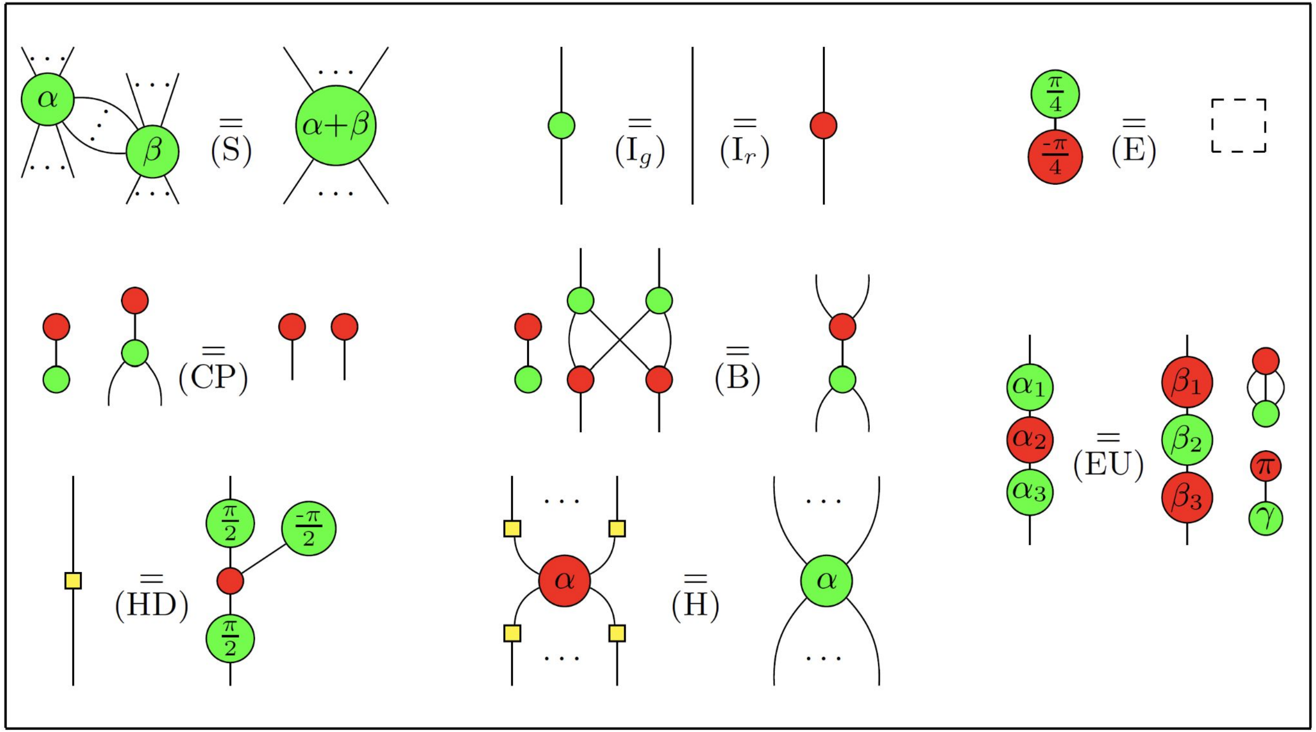
Z spider

X spider



$:= |0\rangle^{\otimes n}\langle 0|^{\otimes m} + e^{i\alpha}|1\rangle^{\otimes n}\langle 1|^{\otimes m}$ and 

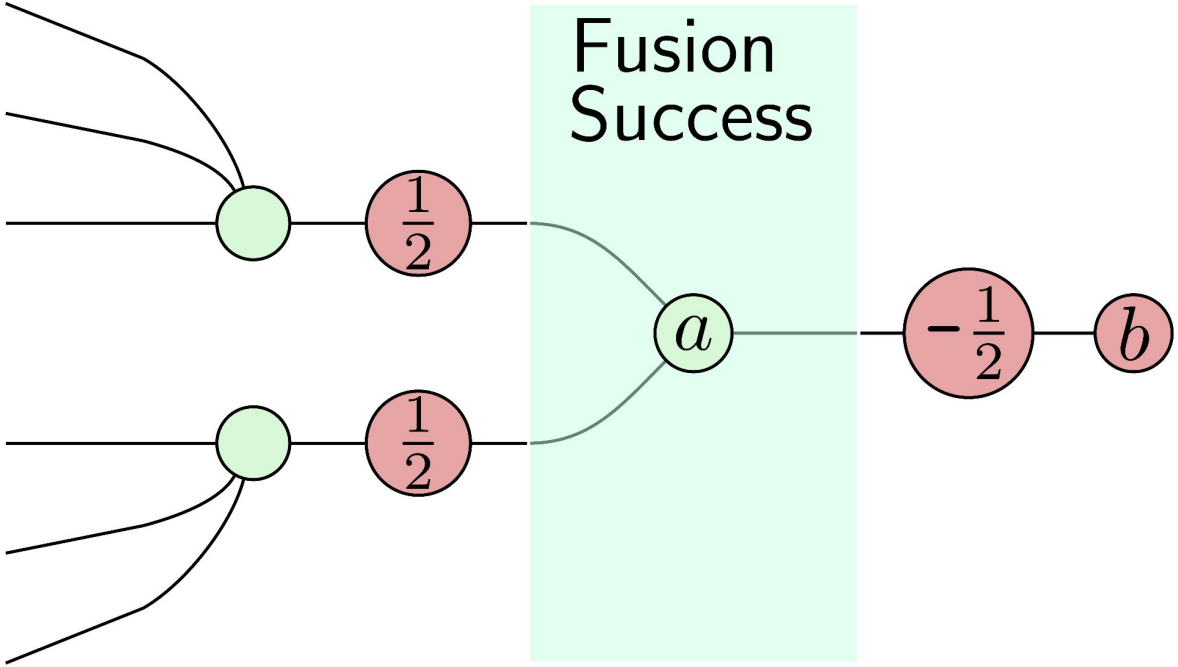
$:= |+\rangle^{\otimes n}\langle +|^{\otimes m} + e^{i\alpha}|-\rangle^{\otimes n}\langle -|^{\otimes m}$



Vilmart doi:10.1109/LICS.2019.8785765

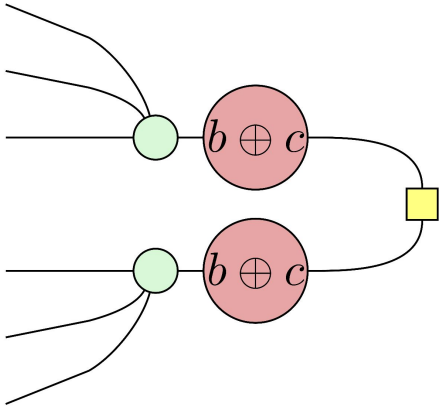
CZ gadget by fusion on cluster states

$$a, b \in \{0, 1\}$$

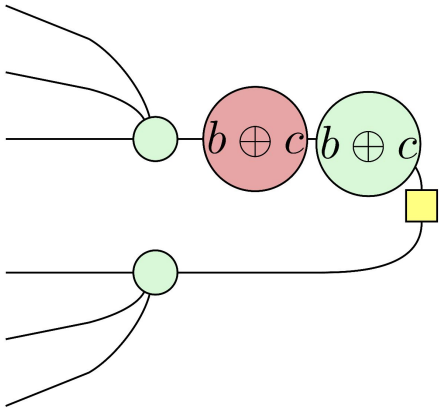


Fusion Measurement Success Case Corrections

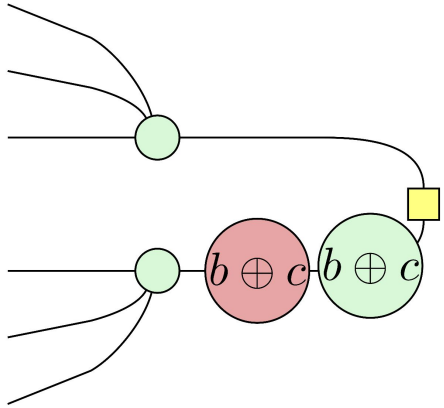
X
X



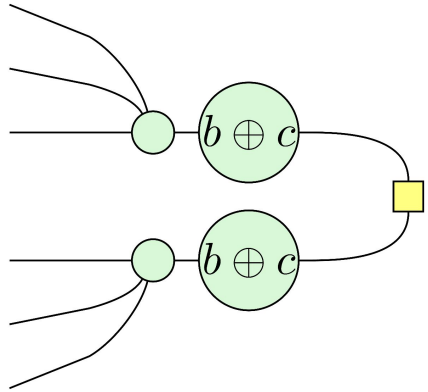
Y
I



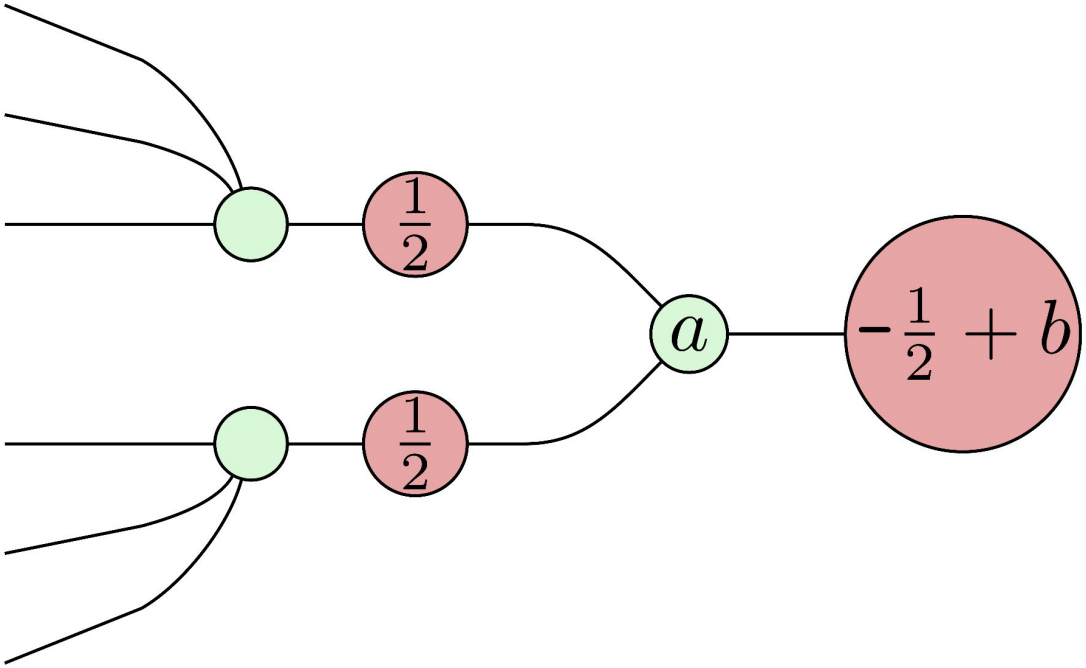
I
Y



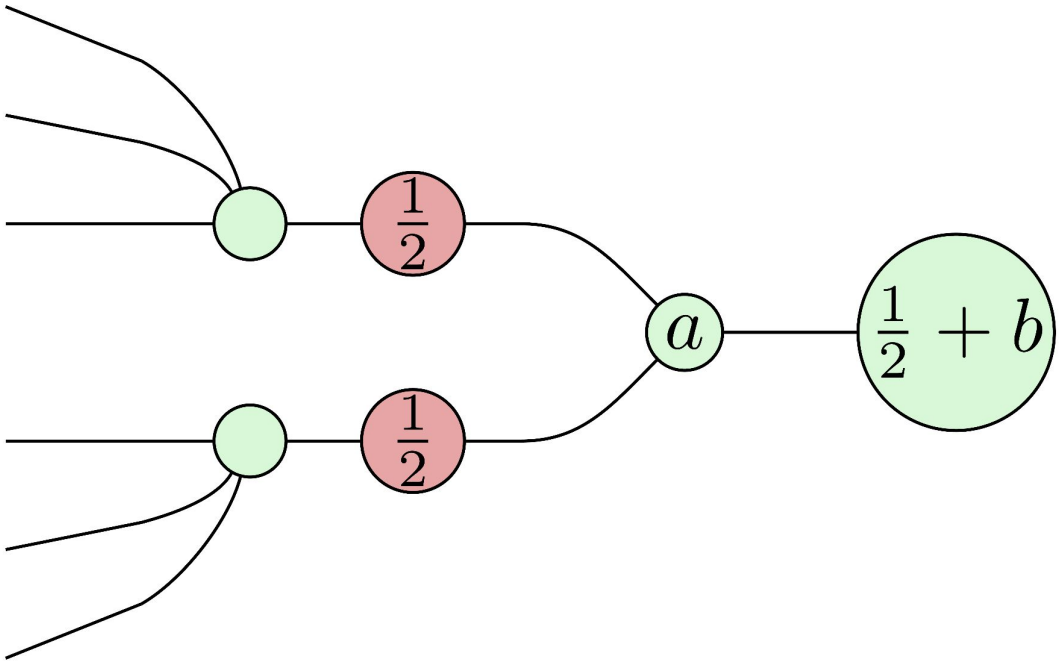
Z
Z



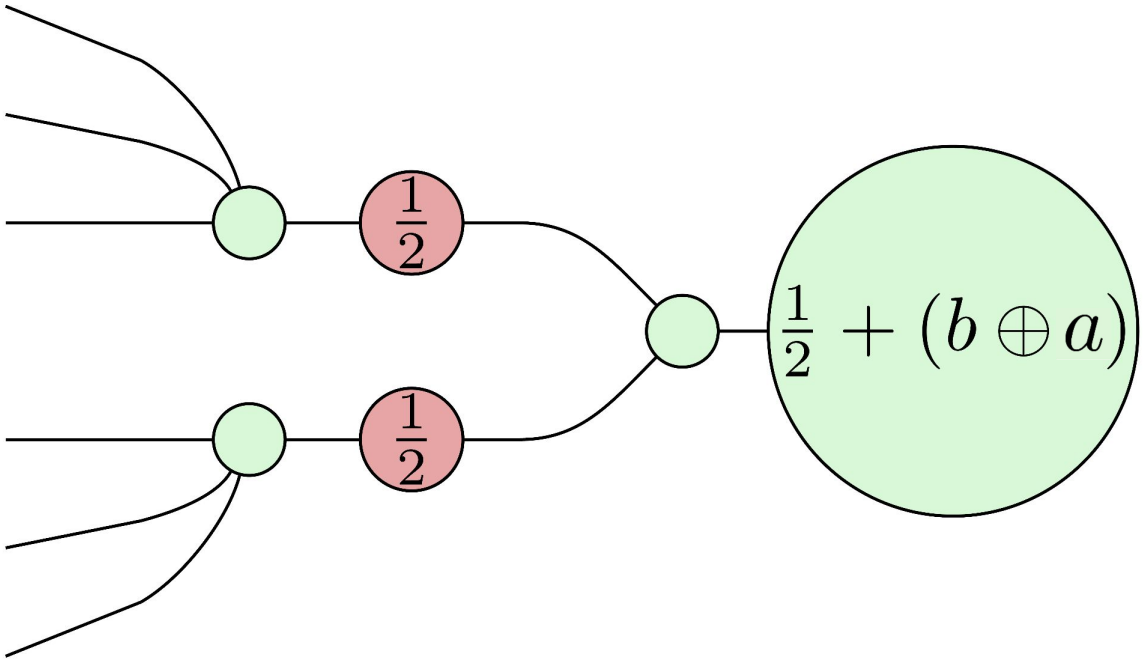
$$a, b \in \{0, 1\}$$



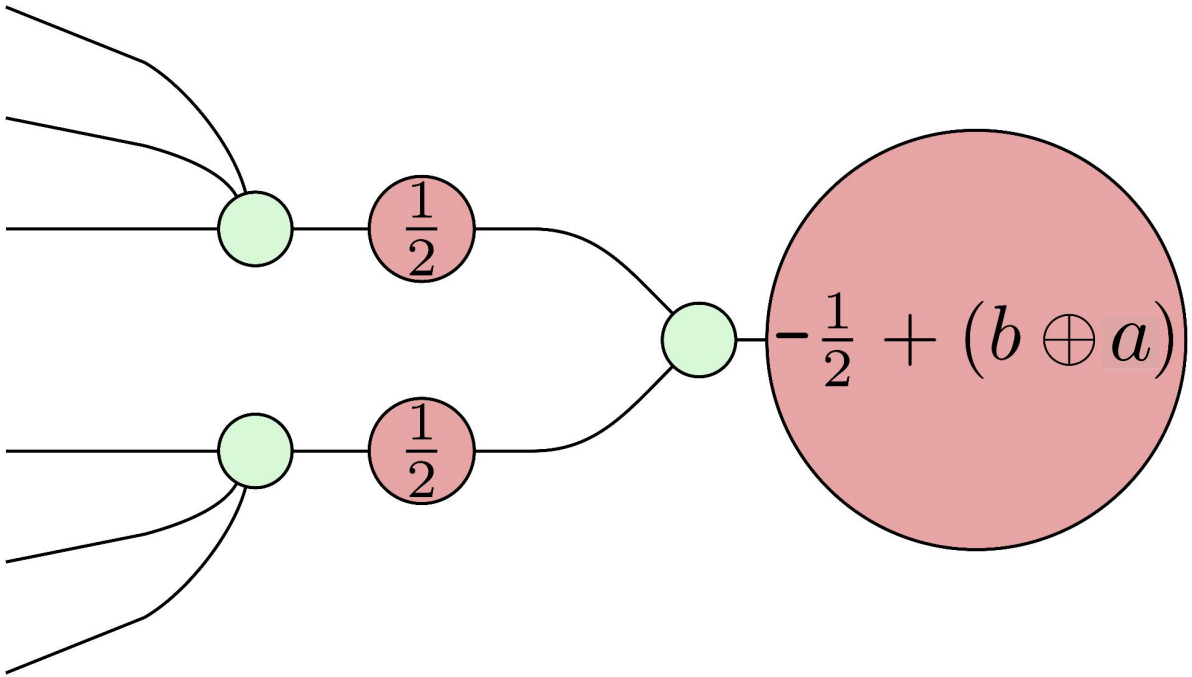
$a, b \in \{0, 1\}$



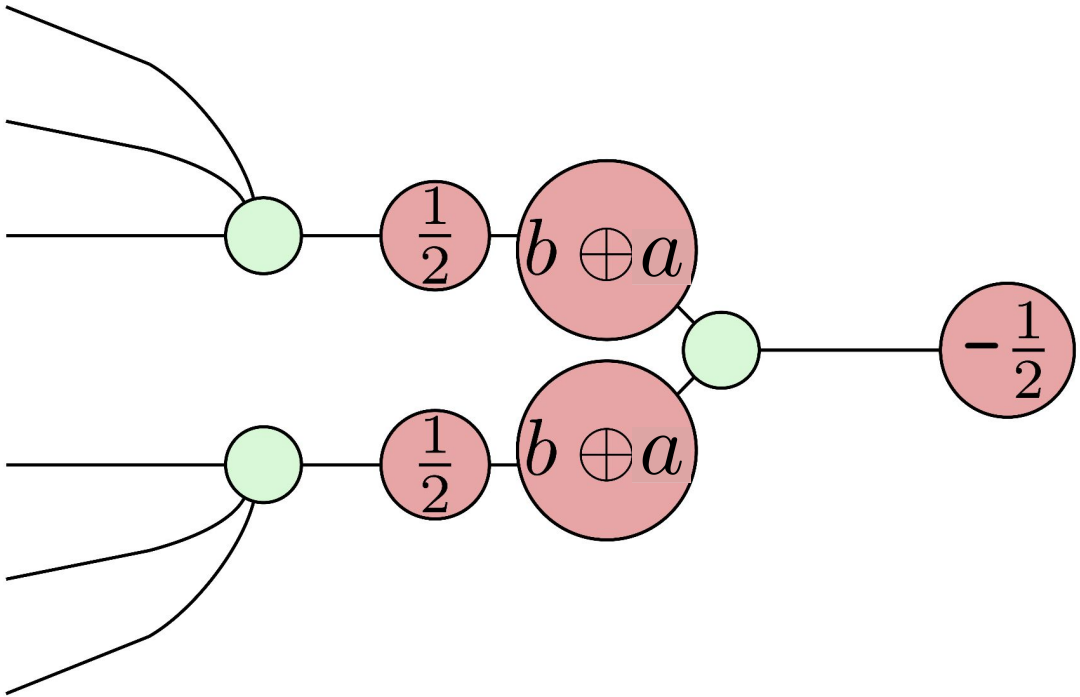
$a, b \in \{0, 1\}$



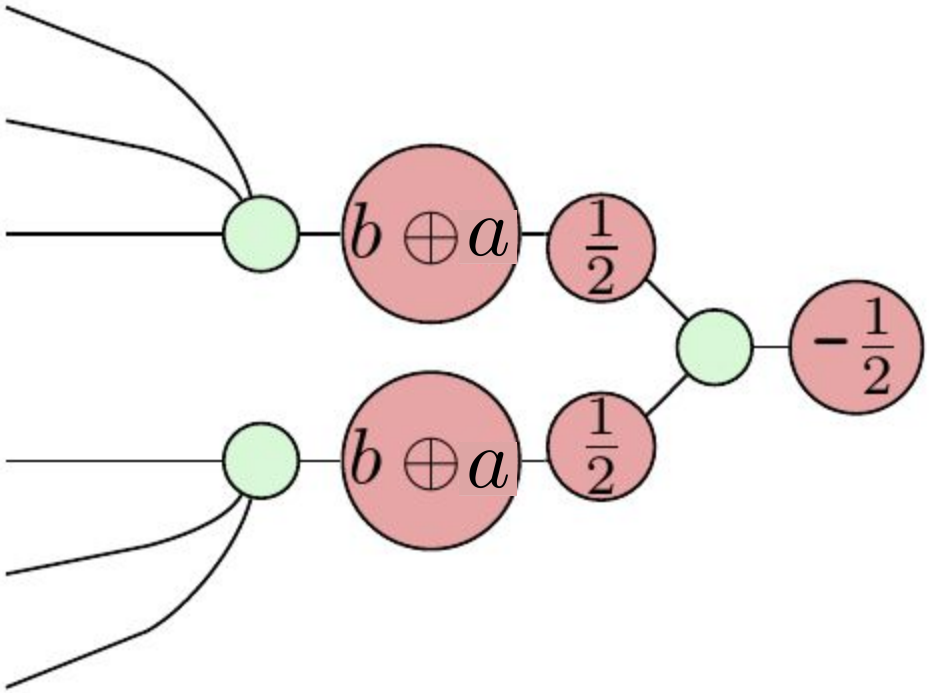
$a, b \in \{0, 1\}$

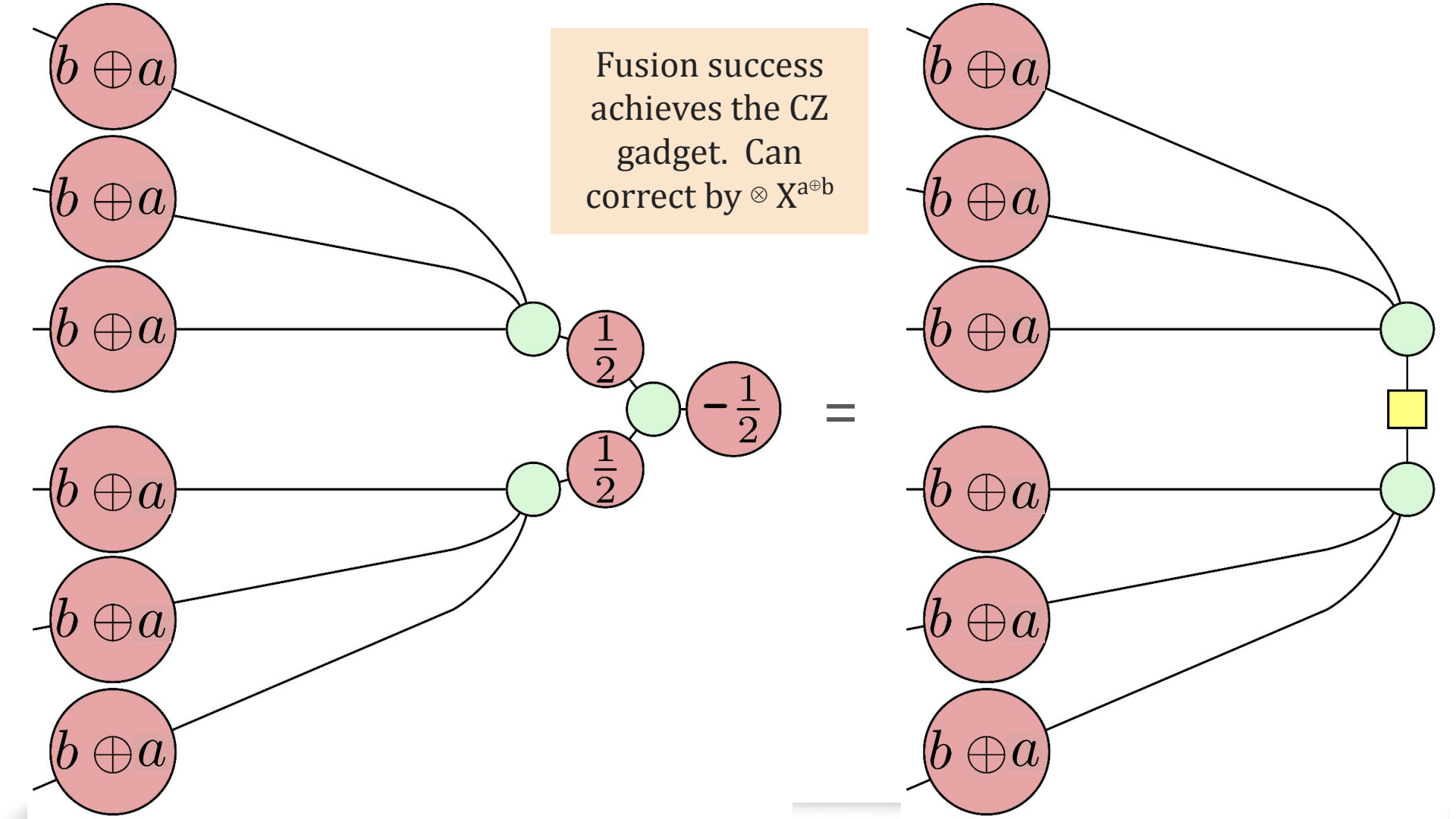


$$a, b \in \{0, 1\}$$

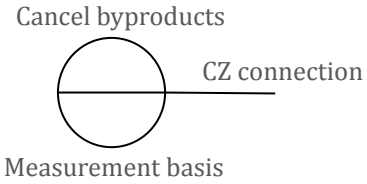


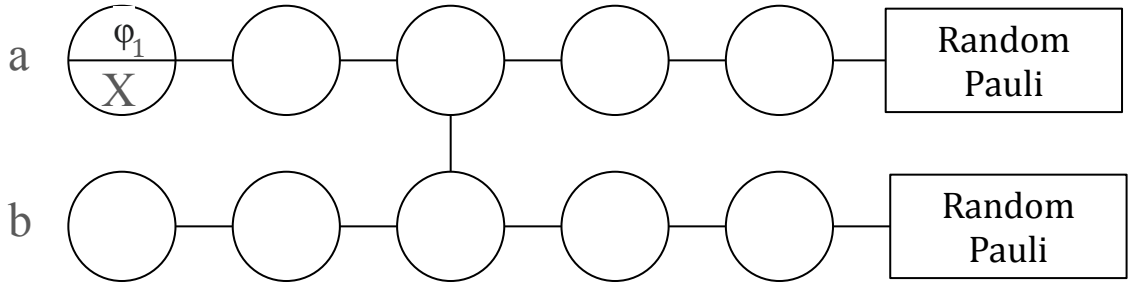
$$a, b \in \{0, 1\}$$

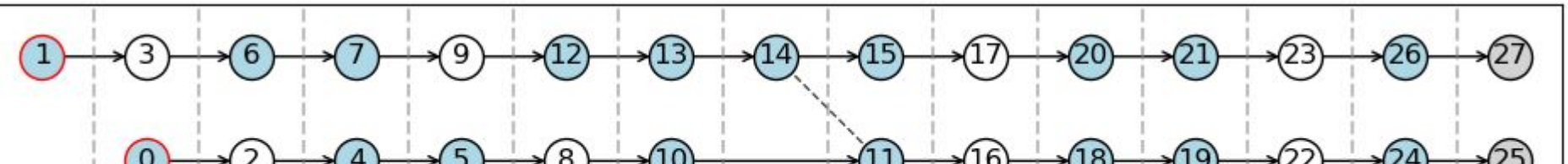



Fusion success achieves the CZ gadget. Can correct by ⊗ X^{a⊕b}
b ⊕ a
b ⊕ a
b ⊕ a
b ⊕ a
b ⊕ a
b ⊕ a
1/2
1/2
−1/2
=
b ⊕ a
b ⊕ a
b ⊕ a
b ⊕ a
b ⊕ a
b ⊕ a

Bonus Challenge: Cluster State Implementation







$$\langle H \rangle = \sum \alpha_{ij} \langle P_i P_j \rangle$$

$$H = \sum \alpha_{ij} P_i P_j$$

$$\phi_1, \phi_2, \cdots, \phi_8$$

$$P_i \in \{I, X, Y, Z\}$$

$$E(\phi_1, \phi_2, \phi_3, \phi_4, \phi_5, \phi_6, \phi_7, \phi_8) = \sum \alpha_{ij} \langle P_i P_j \rangle$$

$$\frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

$$|\psi_{ansatz}\rangle = U(\phi_1, \cdots, \phi_8)|00\rangle$$

$$E(\phi_1, \phi_2, \cdots, \phi_8) = \sum \alpha_{ij} \langle P_i P_j \rangle$$