Classical algorithms for quantum mean values

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Joint work with

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Ramis Movassagh, Eugene Tang

arXiv:1910.08980
arXiv:1909.11485

Simons Institute Workshop
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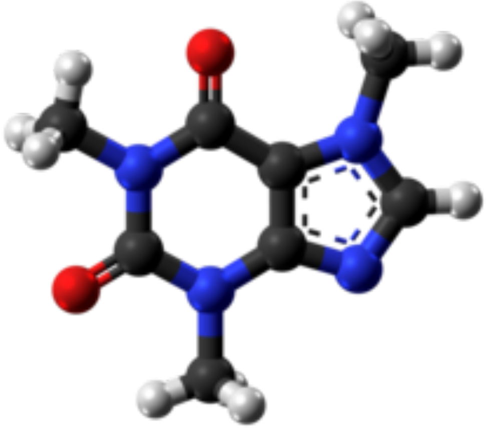
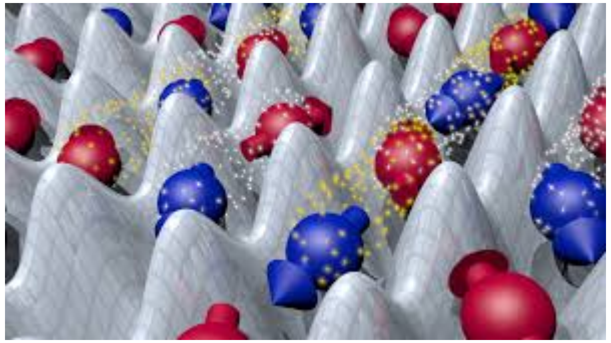
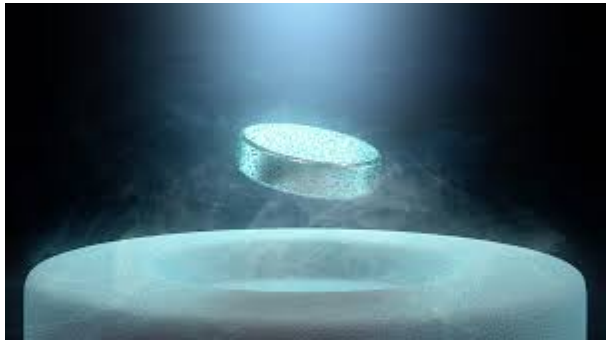
Why quantum many-body problems are hard to solve classically ?

- Exponentially large Hilbert space
- Entanglement
- Sign problem
- Glassiness







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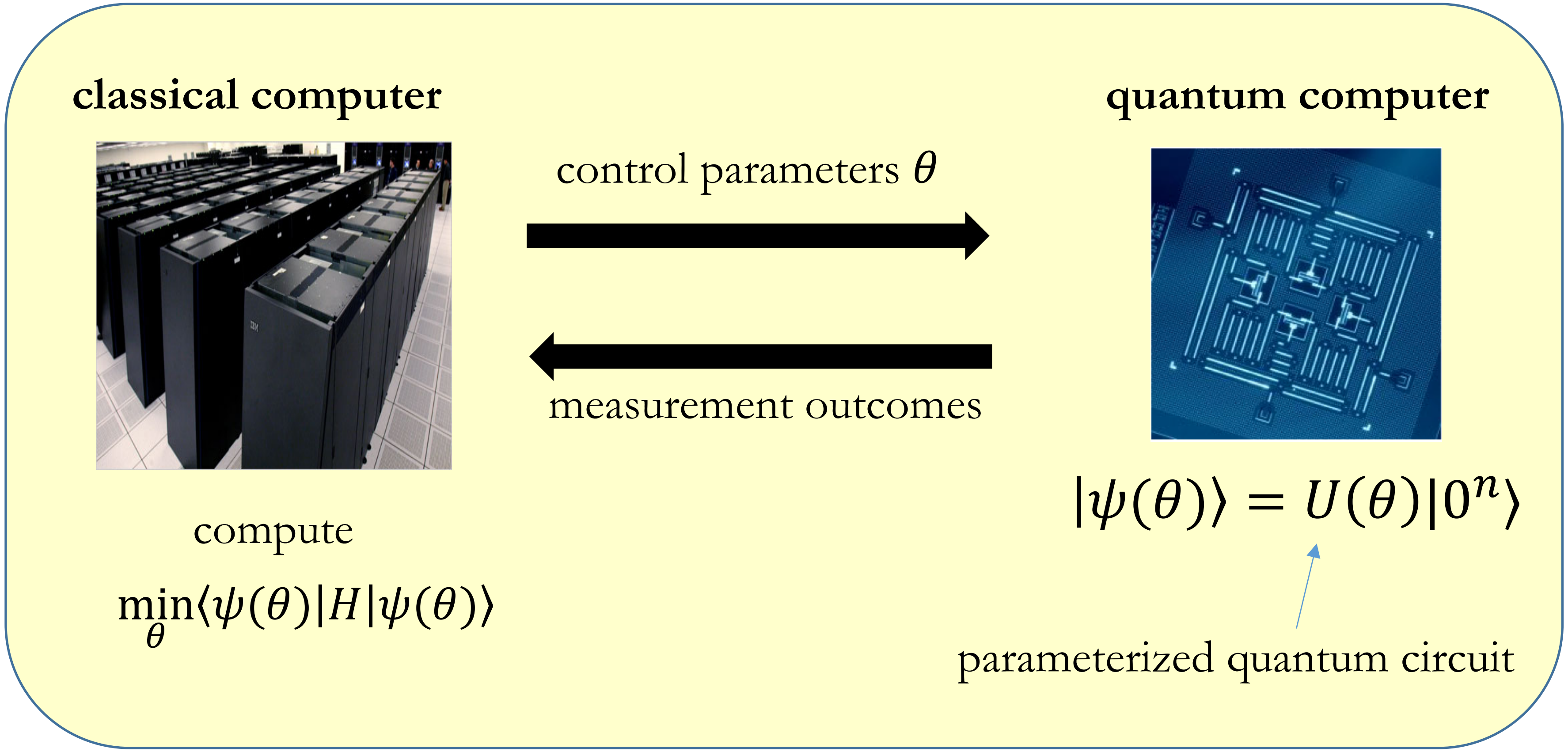
Taming the exponential scaling: **variational algorithms**

Minimize the energy of a Hamiltonian describing a system of n qubits over a class of variational states that depend only on poly(n) parameters.

Variational Quantum Eigensolver (VQE)



classical computer

quantum computer

control parameters θ

measurement outcomes

compute

$\min_{\theta}\langle\psi(\theta)|H|\psi(\theta)\rangle$

$|\psi(\theta)\rangle = U(\theta)|0^n\rangle$

parameterized quantum circuit

nature
THE INTERNATIONAL WEEKLY JOURNAL OF SCIENCE
CHEMICAL SOLUTIONS
Quantum computers extend their reach to solve electronic structures of small molecules
PAGE 242

Simulation of electronic structure in molecules Peruzzo et al 2014, Kandala et al 2017
Quantum Approximate Optimization Algorithm (QAOA) Farhi, Goldstone, Gutmann 2014

Robust agains systematic unitary errors; random errors can be mitigated Temme, SB, Gambetta 2017

Limitations of VQE

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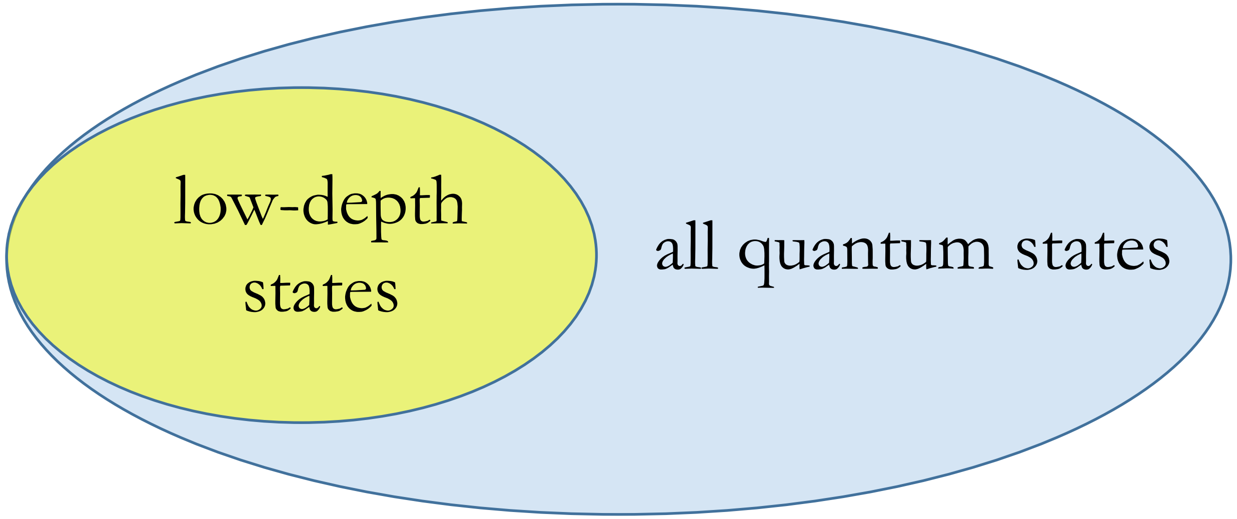
Hardware limitations: depth of the state preparation circuit must be small enough to enable reliable implementation on NISQ devices. Qubit connectivity may be limited, e.g. only 2D or 3D. Highly entangled ground states are out of scope.



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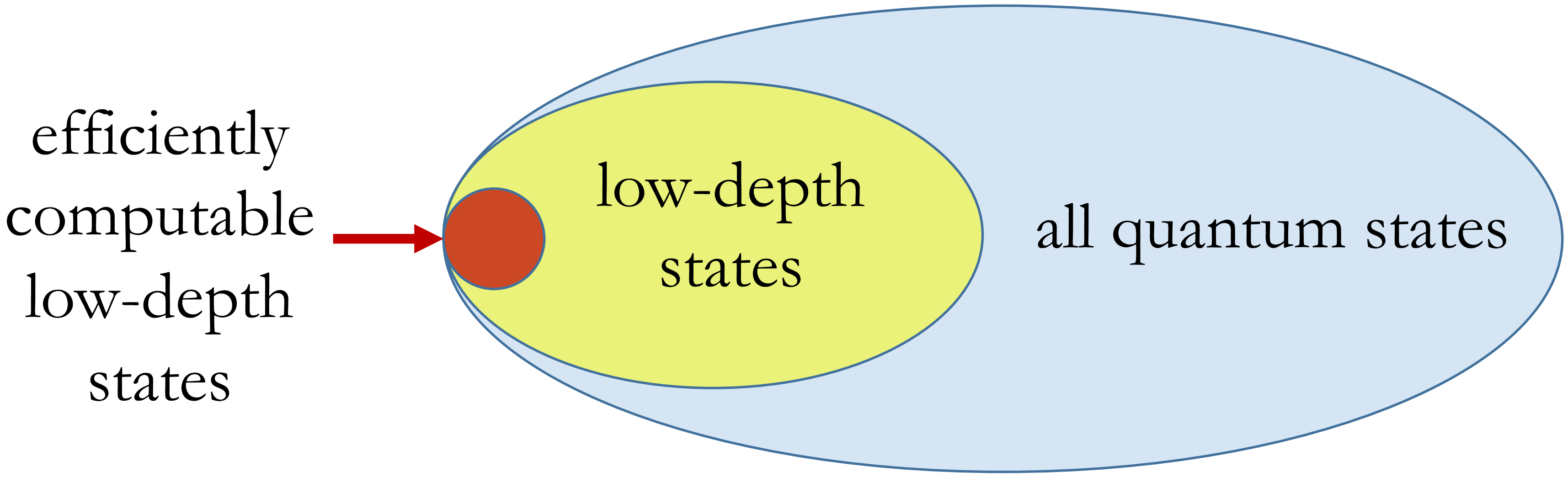
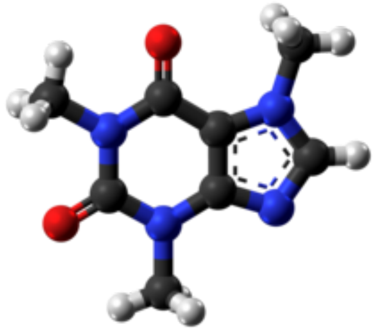
Algorithmic limitations: the number of variational parameters must be small enough to enable efficient energy minimization. Large-scale VQE with an extensive number of variational parameters may give rise to intractable optimization problems.



Variational Quantum Eigensolver (VQE)

Electronic structure simulation for chemistry or material science



2nd quantization

$$t_{\alpha\beta} a_\alpha^+ a_\beta$$

$$u_{\alpha\beta\gamma\delta} a_\alpha^+ a_\beta^+ a_\gamma a_\delta$$

map to qubits

$$H = \sum_{a=1}^{m} c_a P_\alpha$$

$$P_\alpha \in \{I, X, Y, Z\}^{\otimes n}$$

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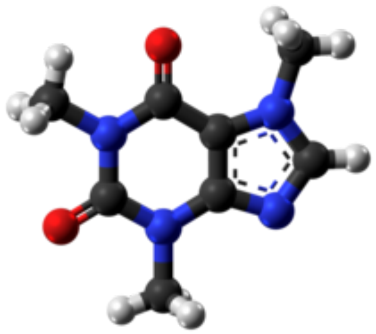

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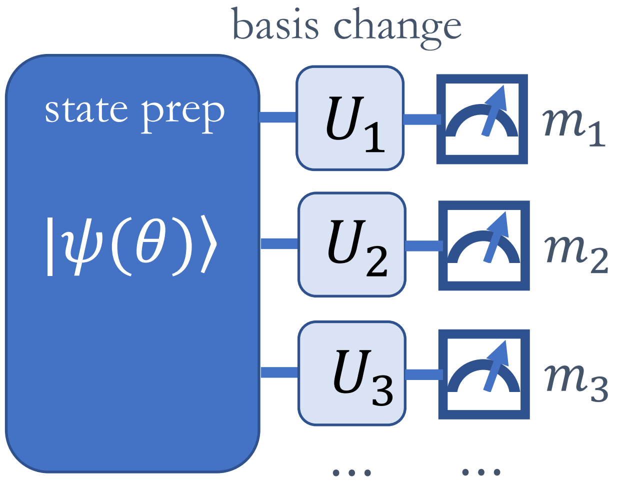
Expected value of a multi-qubit Pauli operator can be inferred by measuring each qubit in X or Y or Z basis and classically multiplying the measured outcomes:

$$\langle\psi(\theta)|X \otimes Y \otimes Z \otimes \cdots|\psi(\theta)\rangle = \underbrace{\mathfrak{E}(-1)^{m_1+m_2+m_3+\cdots}}_{\text{average over many experiments}}$$



Quantum Mean Value problem

Suppose U is a low-depth quantum circuit on n qubits and $\varepsilon > 0$ is the error tolerance. Given a tensor product observable

$$P = P_1 \otimes P_2 \otimes \cdots \otimes P_n, \qquad \|P_i\| \leq 1$$

approximate **QMV** $\equiv \langle 0^n | U^\dagger P U | 0^n \rangle$ within an additive error ε.

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Do we really need a quantum computer to solve the problem ?

Quantum Mean Value problem: classical runtime

variational circuit	best previously known [1,2]	our algorithm
constant depth, 2D	$2^{O(n^{1/2})}$	$O(n\varepsilon^{-2})$
constant depth, 3D	$2^{O(n^{2/3})}$	$\varepsilon^{-2}\, 2^{O(n^{1/3})}$

[1] Aaronson and Chen, arXiv:1612.05903

[2] Markov and Shi, SIAM J. on Comp. (2008), quant-ph/0511069

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No quantum advantage if variational circuits are 2D and constant depth !

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constant depth, all-to-all connectivity	$O(n2^n)$	$2^{\tilde{O}(\sqrt{n \log(1/\varepsilon)})}$

Caveat: we can only compute the magnitude of QMV

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general constant depth	$O(n2^n)$	$2^{\tilde{O}(\sqrt{n \log(1/\varepsilon)})}$

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Aside: inner product algorithm

Van den Nest, "Simulating quantum computers with probabilistic methods", arXiv:0911.1624

$$\langle \Psi_1 | \Psi_2 \rangle = ?$$

Efficient approximation algorithm for computationally tractable states such that

- Amplitudes $\langle x | \Psi_i \rangle$ are easy to compute
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Example: Matrix Product States with a small bond dimension are computationally tractable for any order of qubits.

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The algorithm approximates the inner product with a small additive error.
Computing the inner product exactly or with a small multiplicative error is #P-hard.

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Monte Carlo approach:

$$\langle \Psi_1 | \Psi_2 \rangle = \underbrace{\sum_x |\langle x | \Psi_1 \rangle|^2 \cdot \frac{\langle x | \Psi_2 \rangle}{\langle x | \Psi_1 \rangle}}_{\substack{\text{mean value of a function } f(x) \\ \text{over a distribution } p(x)}}$$

$$Var(f) \leq 1$$

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mean value of a function $f(x)$ over a distribution $p(x)$

$$Var(f) \leq 1$$

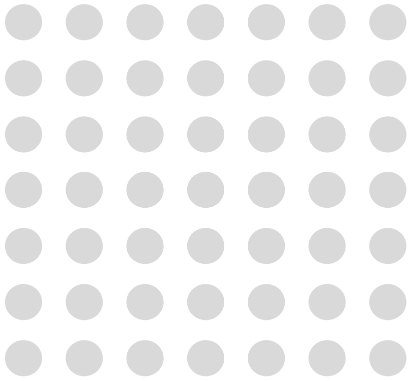
$$\langle \Psi_1 | \Psi_2 \rangle \approx \underbrace{\frac{1}{M} \sum_{i=1}^{M} f(x^i)}$$

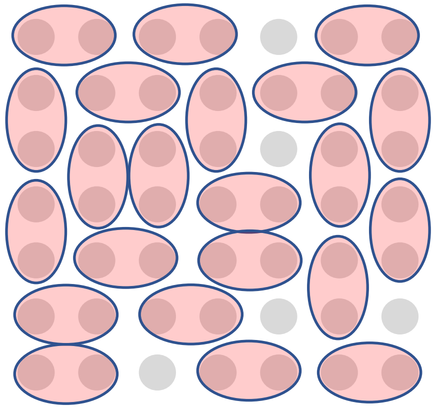
empirical mean value of $f(x)$ over M samples from $p(x)$

Approximation error: $\epsilon \sim M^{-1/2}$

Consider a system of n qubits that live at sites of a 2D grid of size $\sqrt{n}\times\sqrt{n}$

Depth-d circuit U consists of d layers of nearest-neighbor two-qubit gates.





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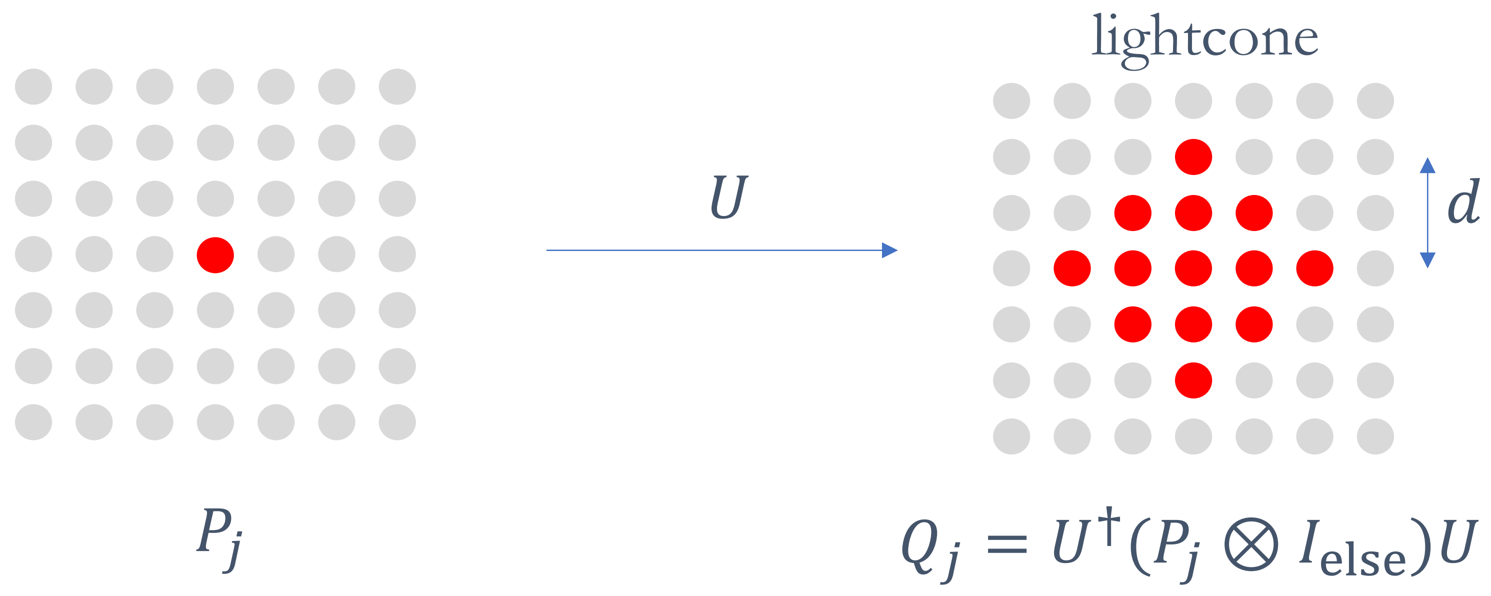
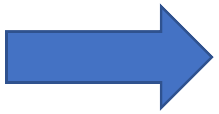


dressed observable

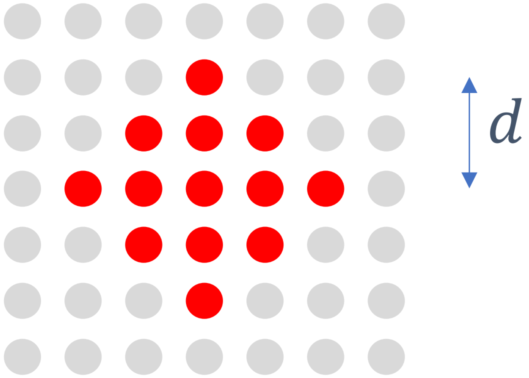
Quantum Mean Value algorithm

Step 1: compute each dressed observable $Q_j = U^\dagger (P_j \otimes I_{\text{else}}) U$



Locality

Simulation within a single light cone



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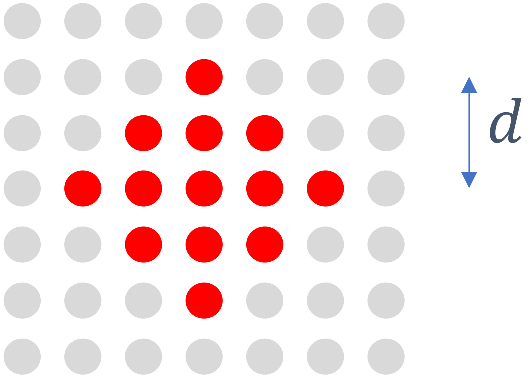
Locality → Simulation within a single light cone

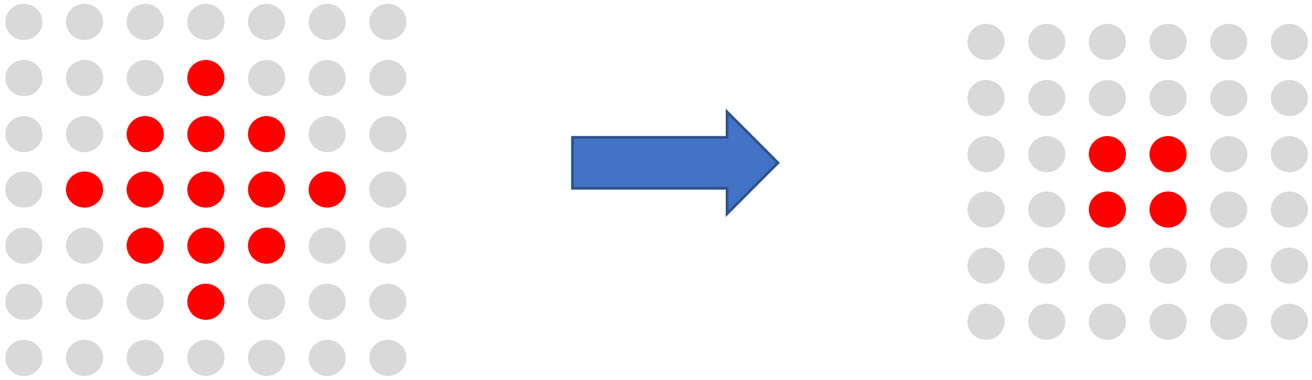


$$Q_i Q_j = Q_j Q_i$$

$$\text{QMV} = \left\langle 0^n \middle| U^\dagger (P_1 \otimes P_2 \otimes \cdots \otimes P_n) U \middle| 0^n \right\rangle = \langle 0^n | Q_1 Q_2 \cdots Q_n | 0^n \rangle$$

Quantum Mean Value algorithm

Step 2: coarse grain the lattice such that each dressed observable Q_i acts on a 2x2 block.



Now each lattice site has local dimension $D = 2^{O(d^2)}$

Quantum Mean Value algorithm

$\text{QMV} = \langle 0^n | Q_1 Q_2 \cdots Q_n | 0^n \rangle$

Q_i act on 2x2 blocks of sites and pairwise commute

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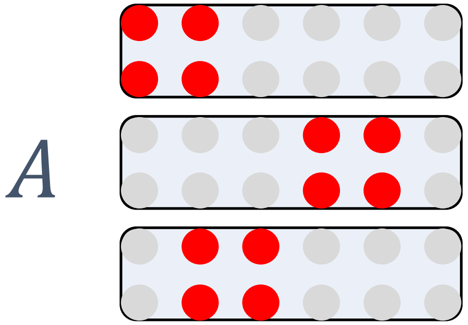
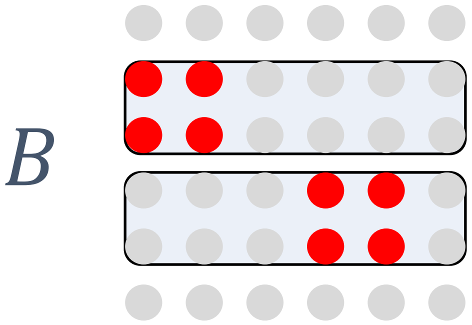
Step 3: reorder the terms to get the inner product of two Matrix Product States (MPS)





$$|\Psi_A\rangle = \prod_{i \in A} Q_i |0^n\rangle$$

$$|\Psi_B\rangle = \prod_{i \in B} Q_i |0^n\rangle$$

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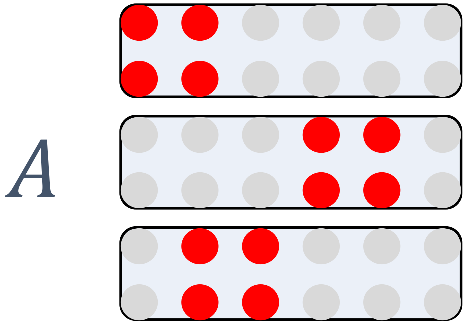

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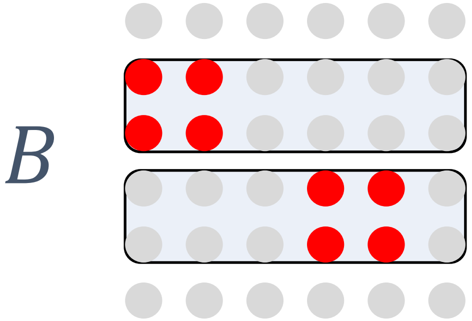


$|\Psi_B\rangle = \prod_{i \in B} Q_i |0^n\rangle$

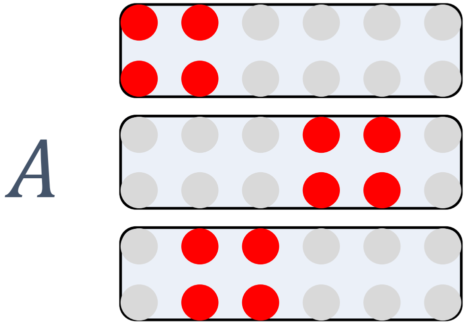
MPS with bond dimension

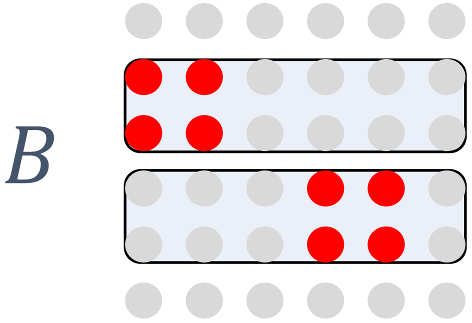
$\chi \leq D^2 = 2^{O(d^2)}$

Quantum Mean Value algorithm

$$\mathrm{QMV} = \langle 0^n | Q_1 Q_2 \cdots Q_n | 0^n \rangle = \langle \Psi_A | W | \Psi_B \rangle$$

permutation of n qubits





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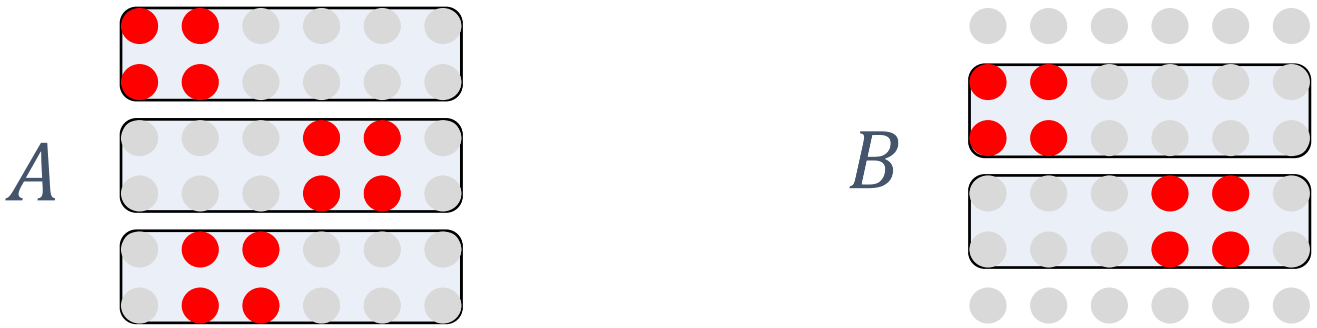
permutation of n qubits

Inner product of computationally tractable states.
Apply Van den Nest algorithm.



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Quantum Approximate Optimization Algorithm [Farhi, Goldstone, Gutmann 2014]

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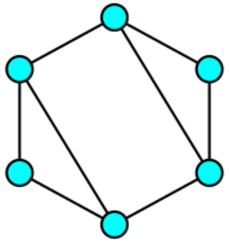
Example: $$C(z) = \sum_{(a,b)\in E} J_{a,b} z_a z_b$$



$G = (V, E)$

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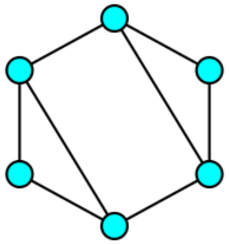

$G = (V, E)$

1) Promote the cost function to a quantum Hamiltonian: $C = \sum_z C(z)|z\rangle\langle z|$

2) Maximize expected energy $\langle\psi|C|\psi\rangle$ over variational states ψ with a few parameters.

3) Measure the optimal state ψ to obtain a classical solution $z \in \{1, -1\}^n$.
Mean value of $C(z)$ equals $\langle\psi|C|\psi\rangle$.

Quantum Approximate Optimization Algorithm [Farhi, Goldstone, Gutmann 2014]

Level-p variational state:

$$|\psi(\beta,\gamma)\rangle = \prod_{j=1}^{p} \exp[-i\beta_j(X_1 + \cdots + X_n)]\exp[-i\gamma_j C]\,|+ + \cdots +\rangle$$

$|+\rangle \sim |0\rangle + |1\rangle$

Variational parameters: $\beta, \gamma \in \mathbb{R}^p$

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Trotterized version of the Adiabatic Quantum Computation for $p = poly(n)$

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Trotterized version of the Adiabatic Quantum Computation for $p = poly(n)$

Reasons for keeping the level p small:

- Non-linear optimization over β and γ is hard
- Need to keep the circuit depth small for near-term implementation

Can low-level QAOA beat classical approximation algorithms for some problem ?

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No-go theorems:

Level-1 QAOA is inferior to local classical optimizers for bounded-degree graphs
[Hastings arXiv:1905.07047]

Level-p QAOA with $p = O(1)$ is inferior to the best known classical approximation algorithm (Goemans-Williamson SDP relaxation) for bounded-degree graphs.
See a talk by Robert Koenig later today

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Can we overcome these limitations ?
New idea: variable elimination and recursive QAOA
[SB, Kliesch, Koenig, Tang, arXiv:1910.08980]

Variable elimination

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1. Run the standard level-p QAOA with cost function that depends on n variables

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We get a new Ising-like cost function $C'(z)$ that depends on $n-1$ variables.

Recursive QAOA

Apply the variable elimination process recursively until only a few variables are left.
Solve the final problem instance by brute force.

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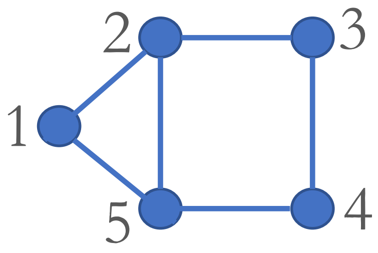

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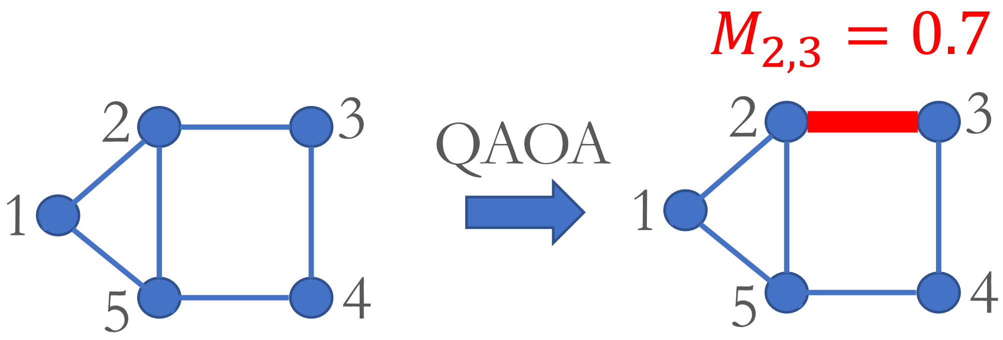
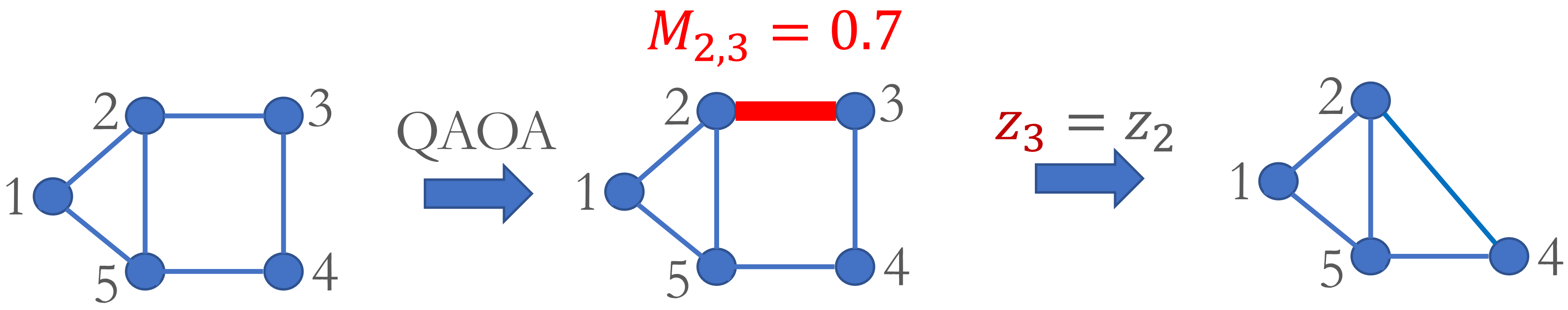


$M_{2,3} = 0.7$

QAOA

Recursive QAOA

Apply the variable elimination process recursively until only a few variables are left.
Solve the final problem instance by brute force.



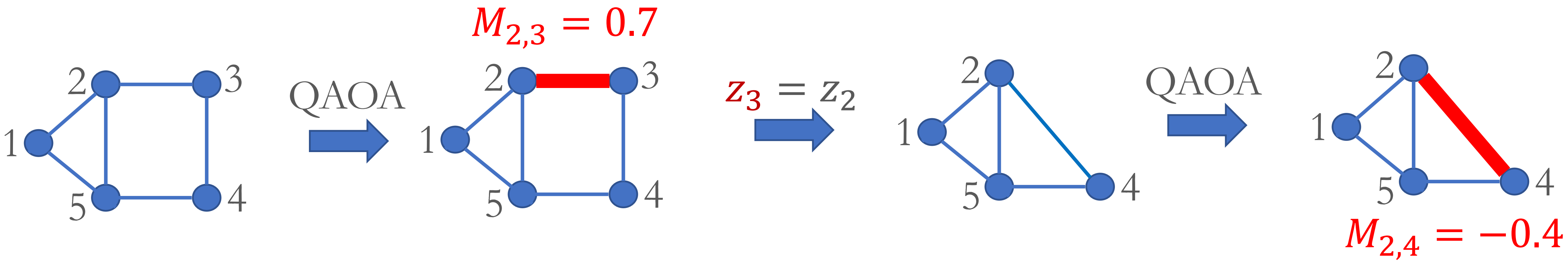
QAOA

$M_{2,3} = 0.7$

$z_3 = z_2$

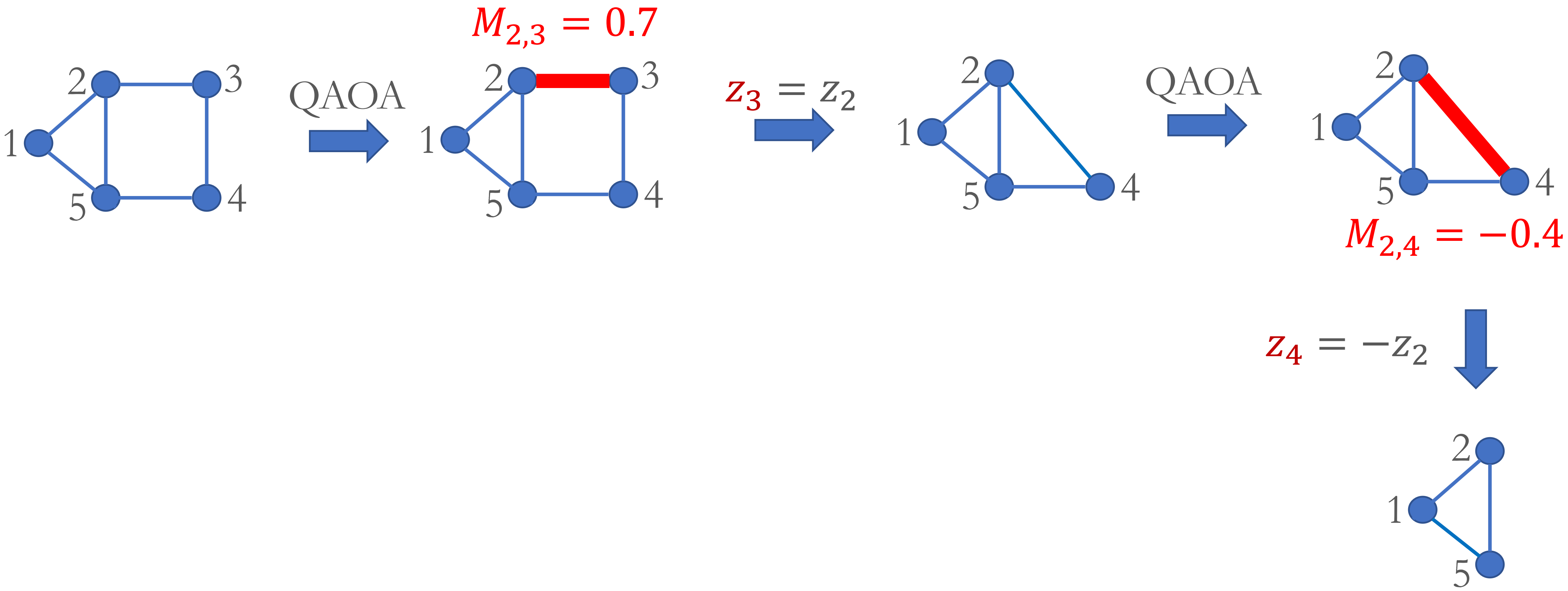
Recursive QAOA

Apply the variable elimination process recursively until only a few variables are left.
Solve the final problem instance by brute force.



Recursive QAOA

Apply the variable elimination process recursively until only a few variables are left.
Solve the final problem instance by brute force.



QAOA

$M_{2,3} = 0.7$

$z_3 = z_2$

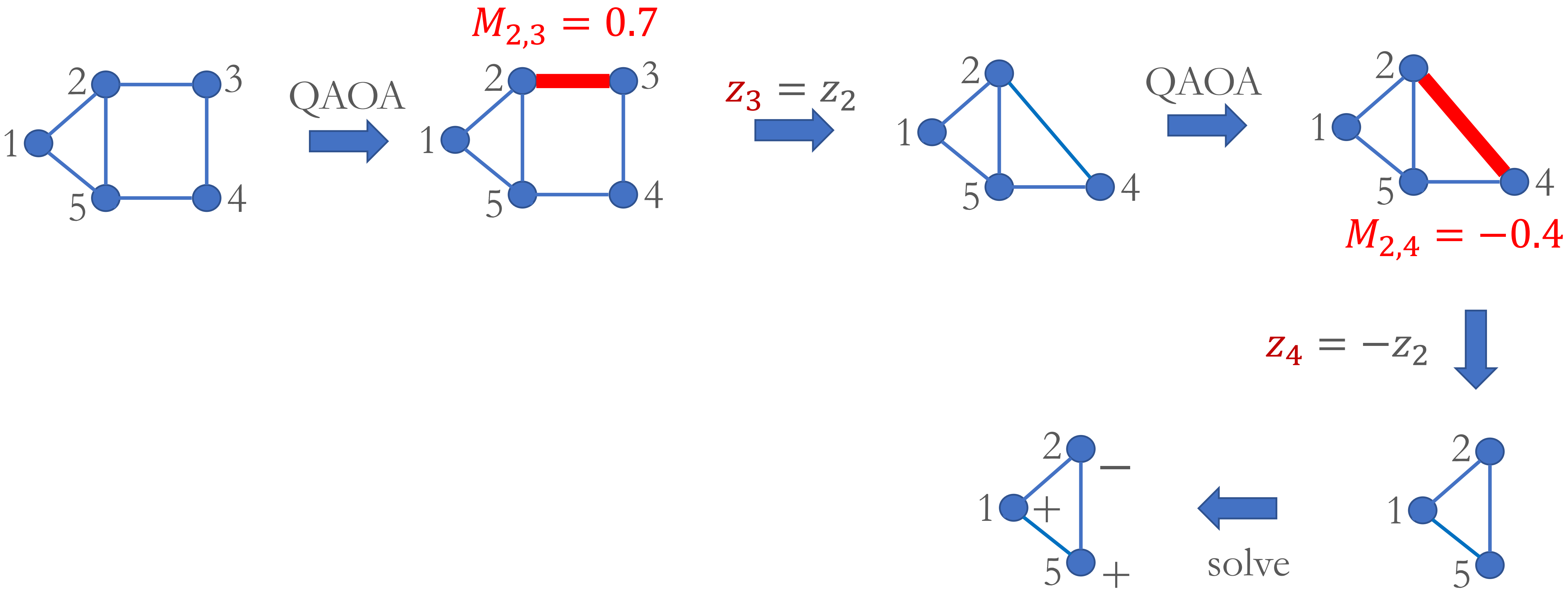
QAOA

$M_{2,4} = -0.4$

$z_4 = -z_2$

Recursive QAOA

Apply the variable elimination process recursively until only a few variables are left.
Solve the final problem instance by brute force.



Recursive QAOA

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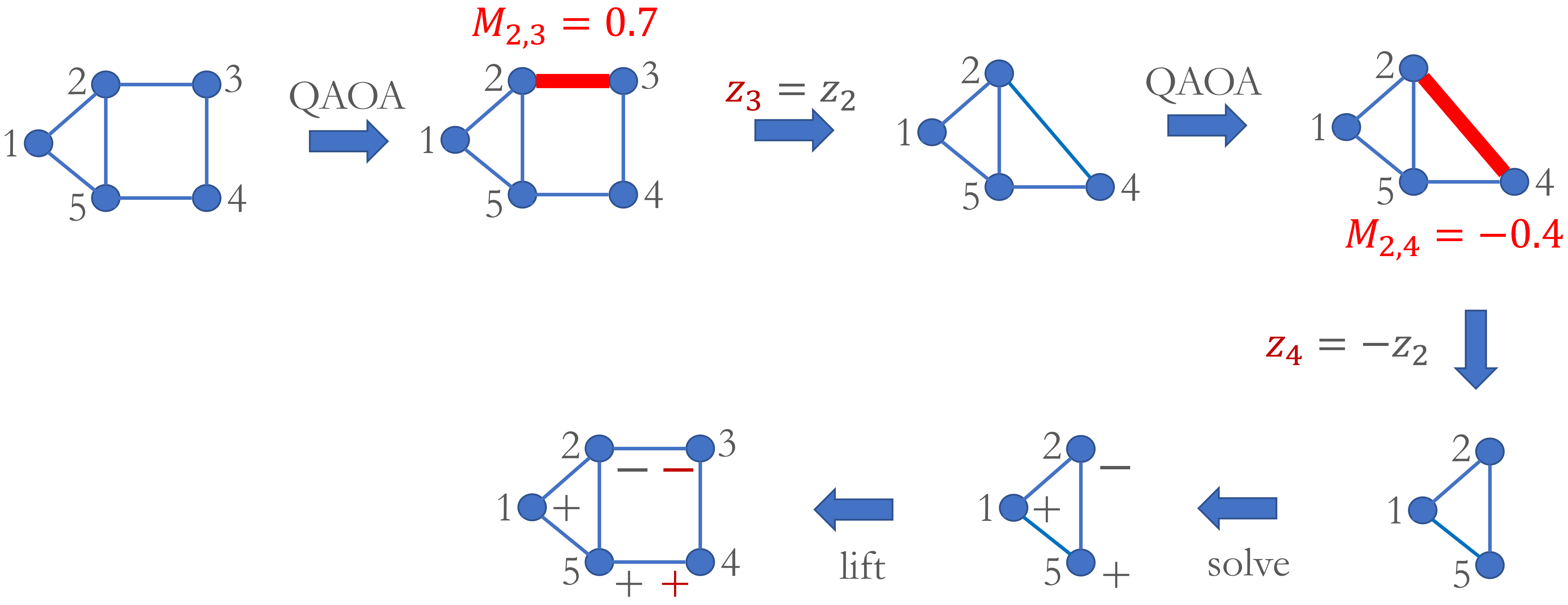
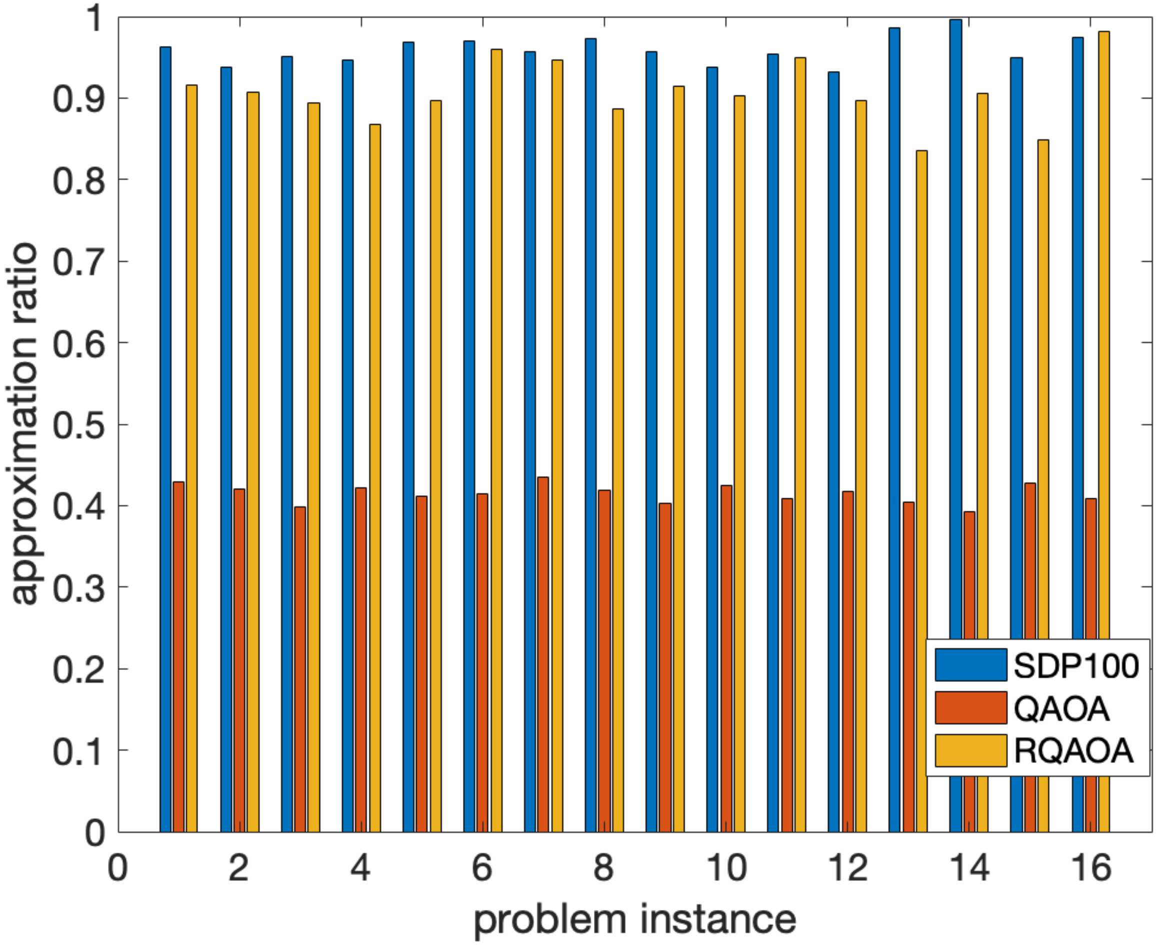


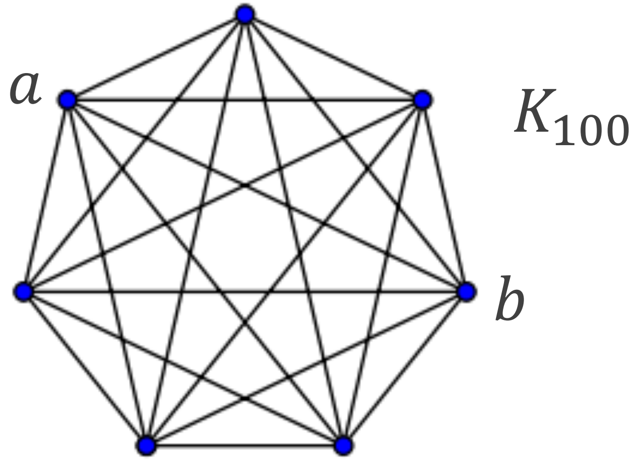
Numerical simulation of level-1 QAOA and RQAOA for 100 qubits.

Cost function: random-bond Ising model on the complete graph.

SDP: Goemans-Williamson semidefinite programming relaxation with 100 rounding trials.



$$C(z) = \sum_{a<b} J_{a,b} z_a z_b$$



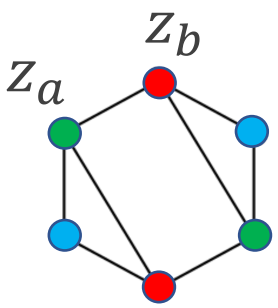
$J_{a,b} \in \mathrm{N}(0,1)$

MAX 3-CUT problem

MAX 3-CUT problem

Variables: vertex colors $z_a \in \{0,1,2\}$

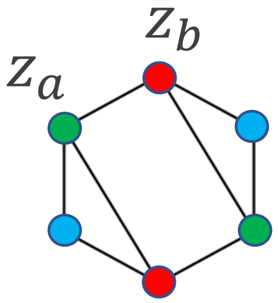
Cost function: $C(z) = \#\{\text{edges } (a,b) : z_a \neq z_b\}$



$G = (V, E)$

MAX 3-CUT problem

Variables: vertex colors $z_a \in \{0,1,2\}$



$G = (V, E)$

Cost function: $C(z) = \#\{\text{edges } (a,b) : z_a \neq z_b\}$

Goal: approximate $C_{max} = \max_z C(z)$

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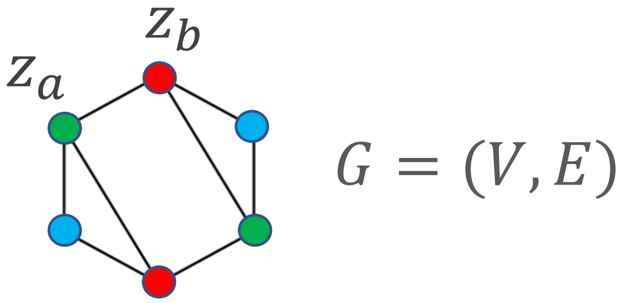

Variables: vertex colors $z_a \in \{0, 1, 2\}$

Cost function: $C(z) = \#\{\text{edges } (a, b) : z_a \neq z_b\}$

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Random guessing: $C(z) \geq \left(\frac{2}{3}\right) C_{max}$

MAX 3-CUT problem

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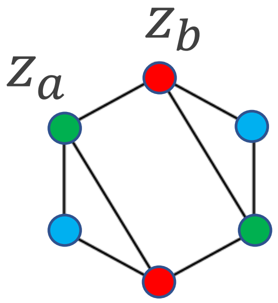

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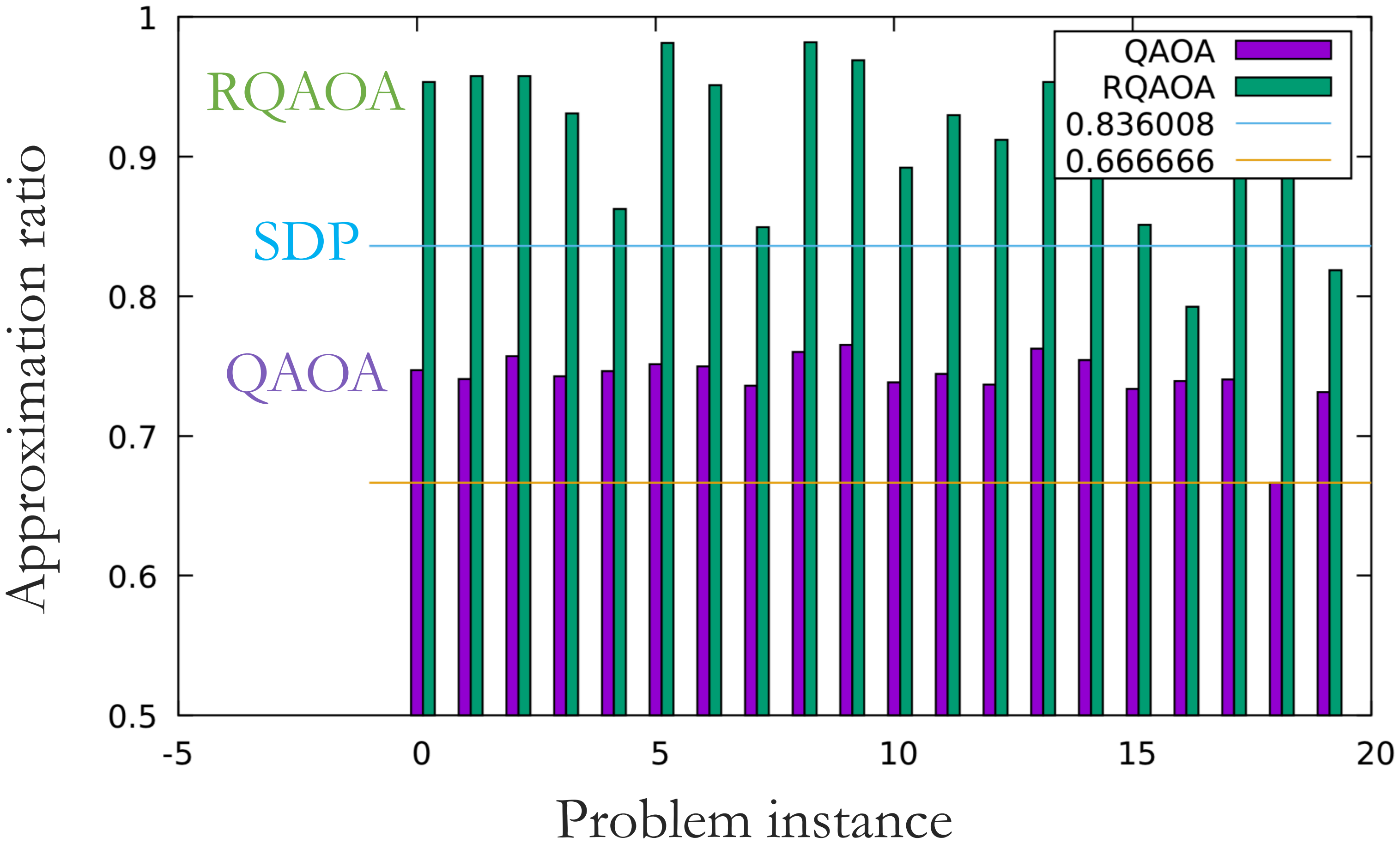
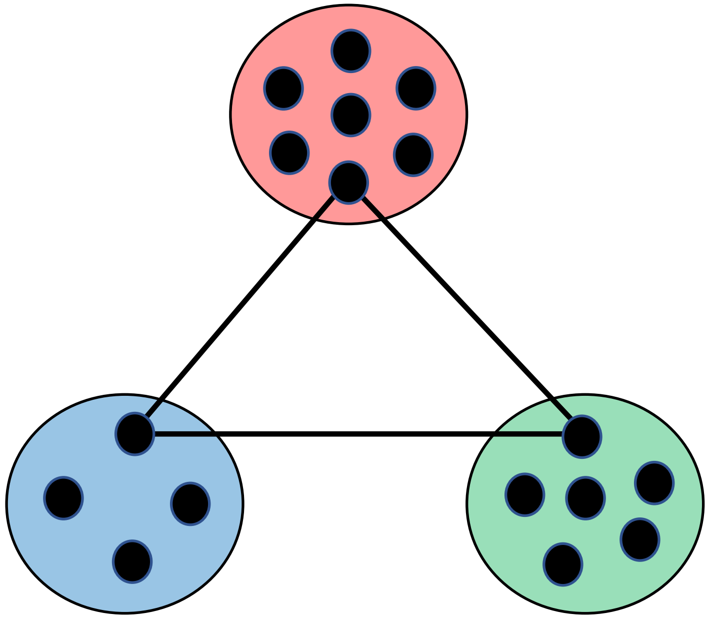
Goal: approximate $C_{max} = \max_z C(z)$

Random guessing: $C(z) \geq \left(\frac{2}{3}\right) C_{max}$

SDP relaxation algorithm: $C(z) \geq 0.836 \cdot C_{max}$
[Klerk, Pasechnik, Warners 2004]

Numerical simulations of level-1 QAOA and RQAOA for 50 qutrits and the MAX 3-CUT cost function. We consider a random ensemble of 3-colorable dense graphs with 50 vertices randomly partitioned into red/blue/green.





add random red-blue, red-green, blue-green edges with probability ½ for each pair of vertices

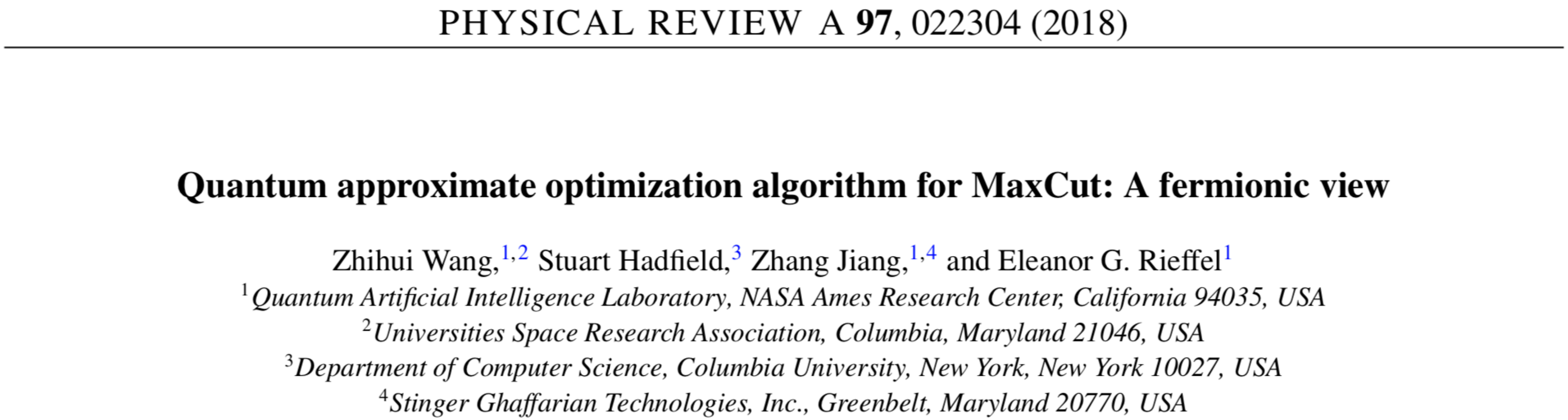
Bad news: **no quantum advantage for level-1 RQAOA**

Bad news: **no quantum advantage for level-1 RQAOA**

The only "quantum" step: computing quantum mean values

$$M_{a,b} = \langle \psi(\beta,\gamma) | Z_a Z_b | \psi(\beta,\gamma) \rangle$$

Efficient classical algorithm for level-1 QAOA



PHYSICAL REVIEW A **97**, 022304 (2018)

Quantum approximate optimization algorithm for MaxCut: A fermionic view

Zhihui Wang,[1,2] Stuart Hadfield,[3] Zhang Jiang,[1,4] and Eleanor G. Rieffel[1]

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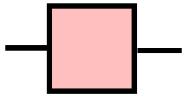
[2] *Universities Space Research Association, Columbia, Maryland 21046, USA*

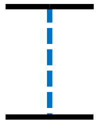
[3] *Department of Computer Science, Columbia University, New York, New York 10027, USA*

[4] *Stinger Ghaffarian Technologies, Inc., Greenbelt, Maryland 20770, USA*

Quantum Mean Value problem for level-1 QAOA

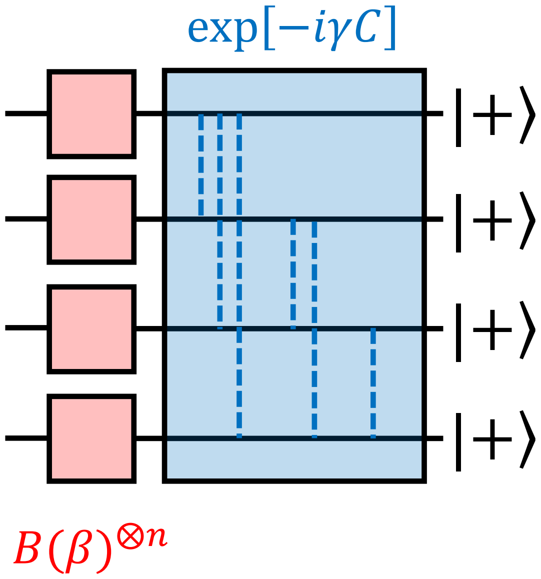


X-rotation



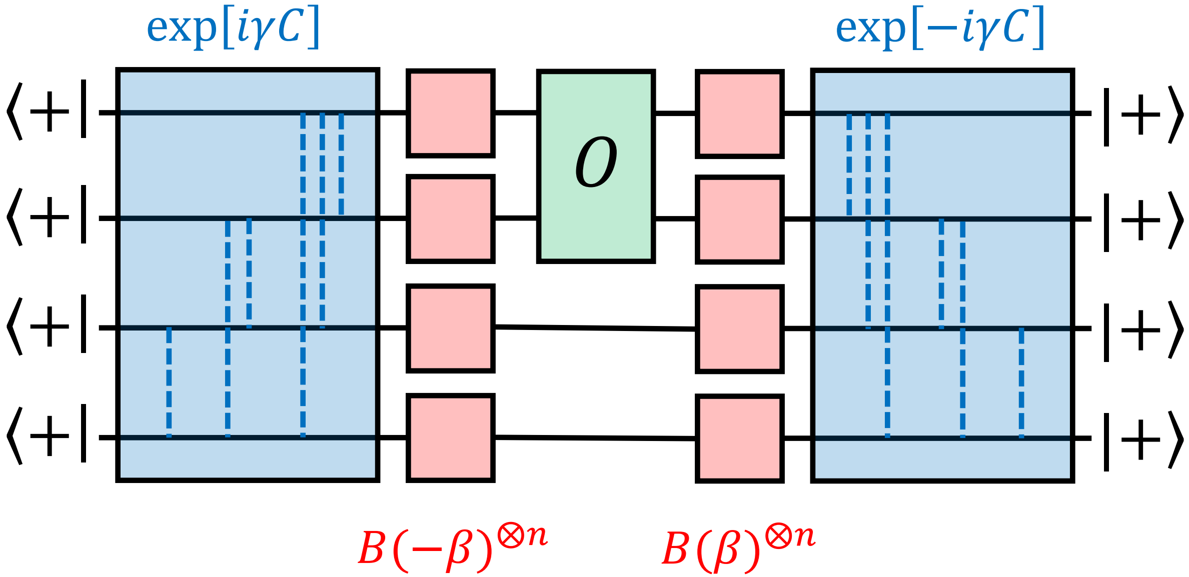
Diagonal two-qudit gate

$$|\psi(\beta,\gamma)\rangle =$$



Quantum Mean Value problem for level-1 QAOA

$$\mathrm{QMV} = \langle \psi(\beta,\gamma) | O_{1,2} | \psi(\beta,\gamma) \rangle =$$



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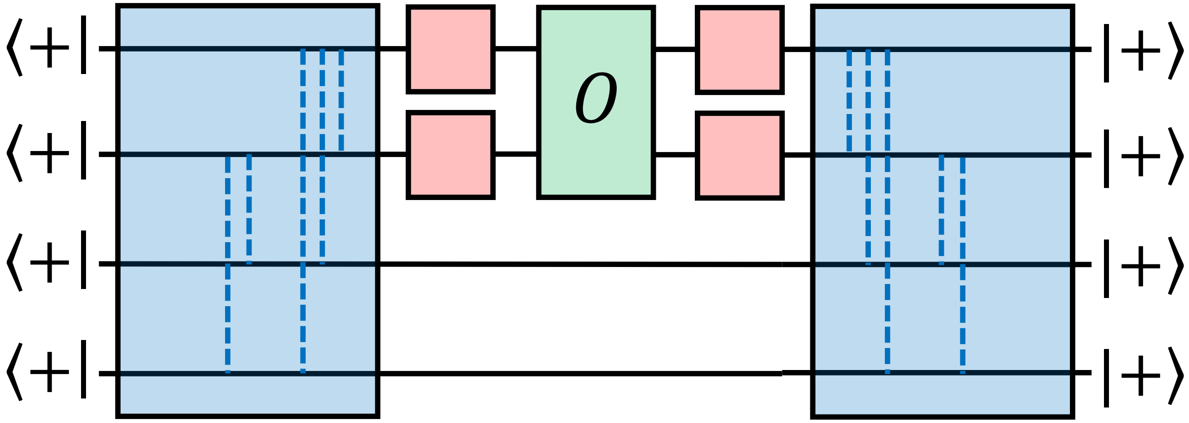
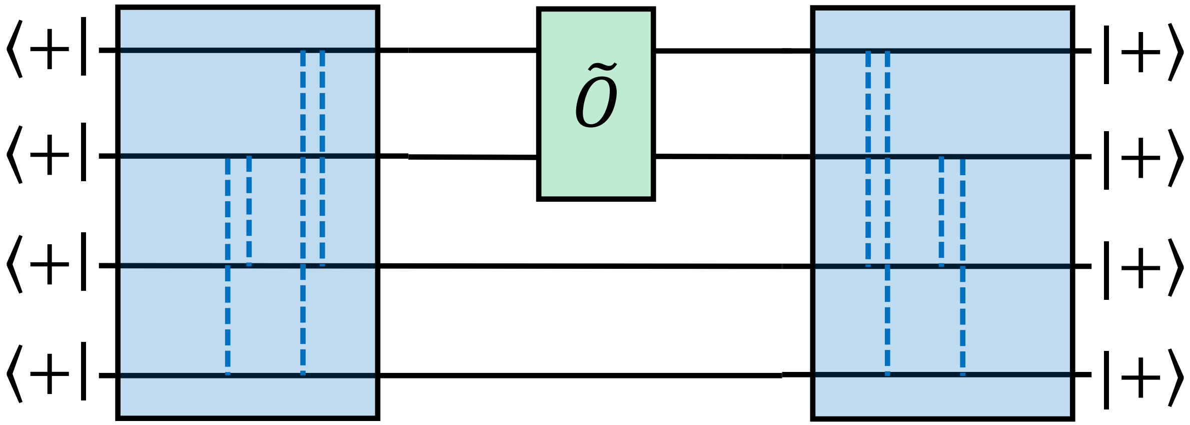


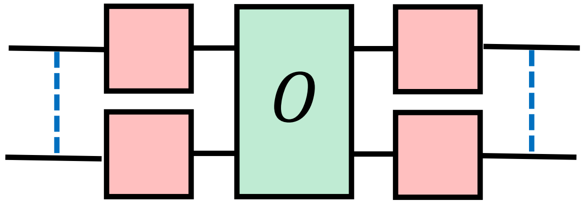
Cancel all gates that do not touch qudits 1,2

Quantum Mean Value problem for level-1 QAOA

$$\mathrm{QMV} = \langle \psi(\beta,\gamma) | O_{1,2} | \psi(\beta,\gamma) \rangle =$$

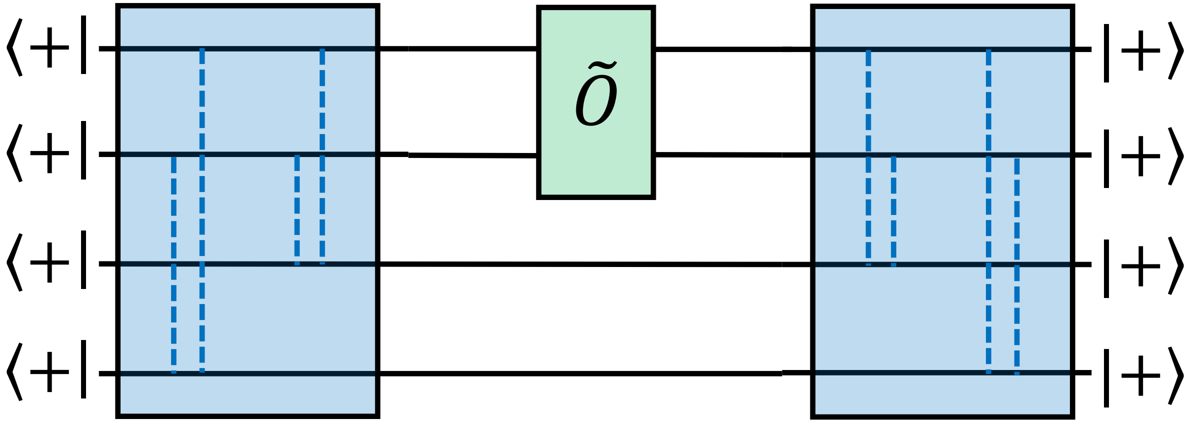


$$\tilde{O} =$$



Quantum Mean Value problem for level-1 QAOA

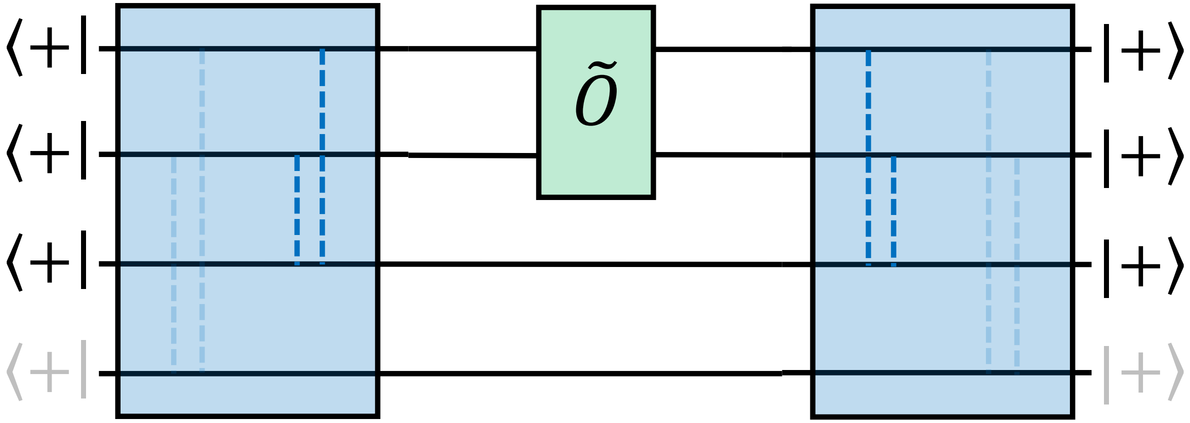
$$\mathrm{QMV} = \langle \psi(\beta,\gamma) | O_{1,2} | \psi(\beta,\gamma) \rangle =$$



Change the order of gates such that qudits 1,2 are coupled to qudits 3,4,…,n sequentially.

Quantum Mean Value problem for level-1 QAOA

$$\mathrm{QMV} = \left\langle \psi(\beta,\gamma) \middle| O_{1,2} \middle| \psi(\beta,\gamma) \right\rangle =$$



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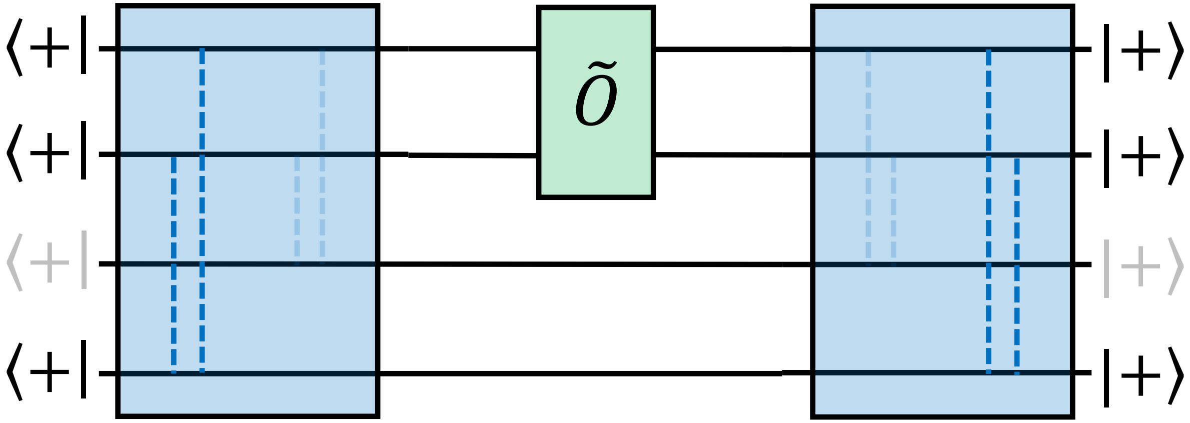
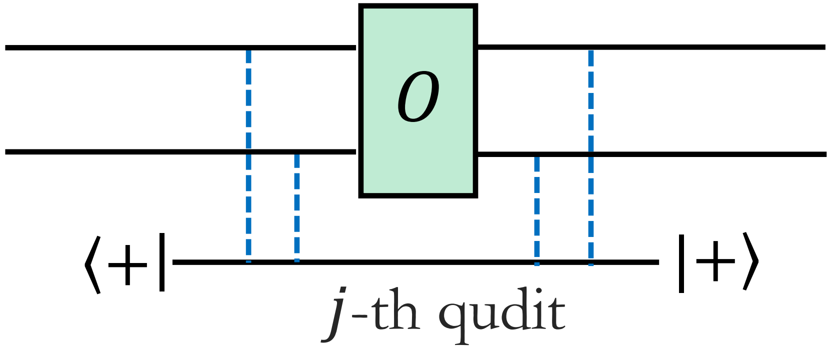


Change the order of gates such that qudits 1,2 are coupled to qudits 3,4,…,n sequentially.

Quantum Mean Value problem for level-1 QAOA

$$\mathtt{QMV} = \langle\psi(\beta,\gamma)|O_{1,2}|\psi(\beta,\gamma)\rangle = \langle + +|\Phi_n \circ \Phi_{n-1} \circ \cdots \circ \Phi_3(\tilde{O})|+ +\rangle$$

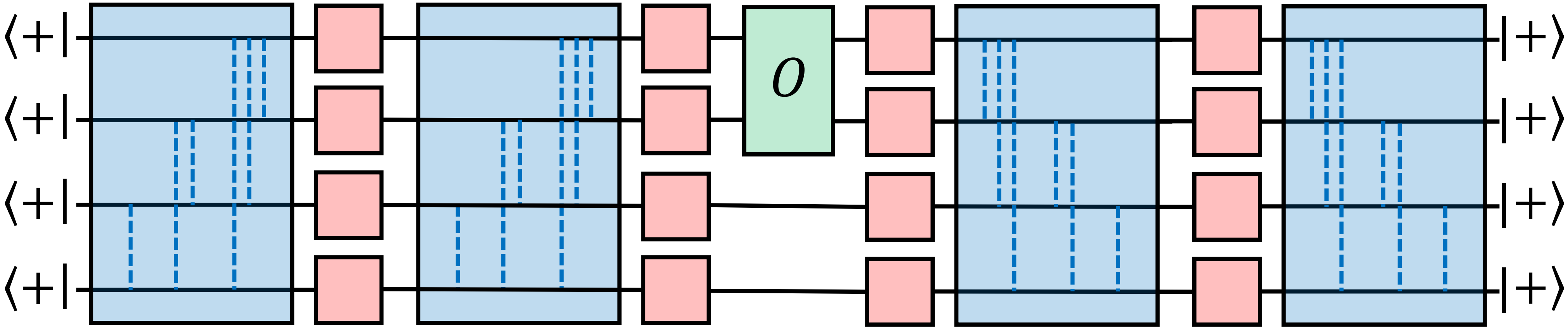
$\Phi_j(O) =$



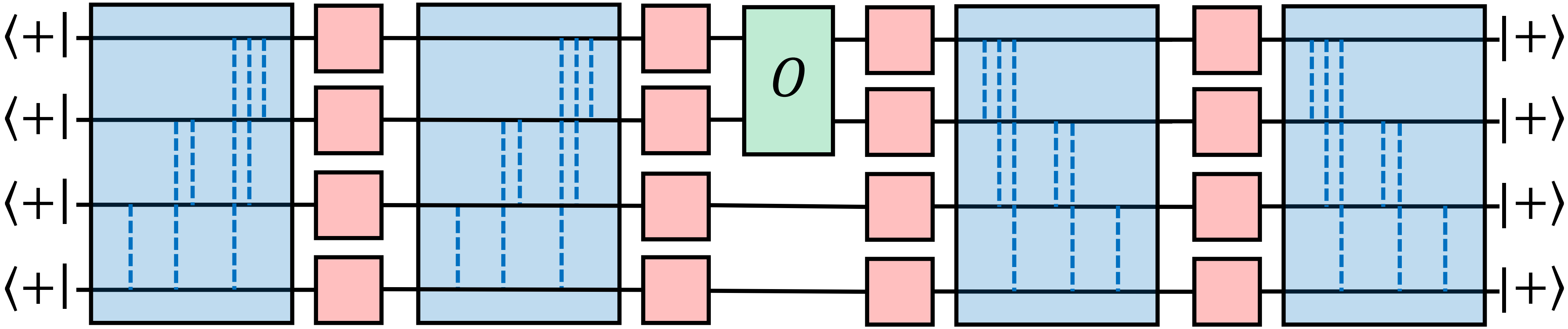
Sequential coupling: need to compute a product of two-qudit quantum channels.
Classical simulation time $O(n)$ assuming that qudit dimension is $O(1)$.

Quantum Mean Value problem for level-2 QAOA

Quantum Mean Value problem for level-2 QAOA



Quantum Mean Value problem for level-2 QAOA

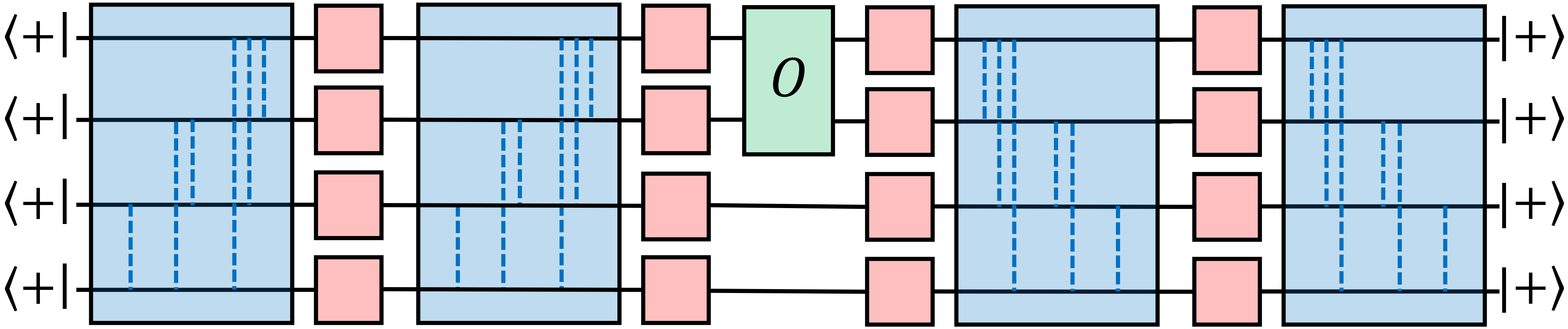


Our algorithm:

Arbitrary interaction graph: runtime $2^{n/2}\epsilon^{-2}$

Planar interaction graph: runtime $O(n^2\epsilon^{-2})$. Works for qudits of constant dimension.

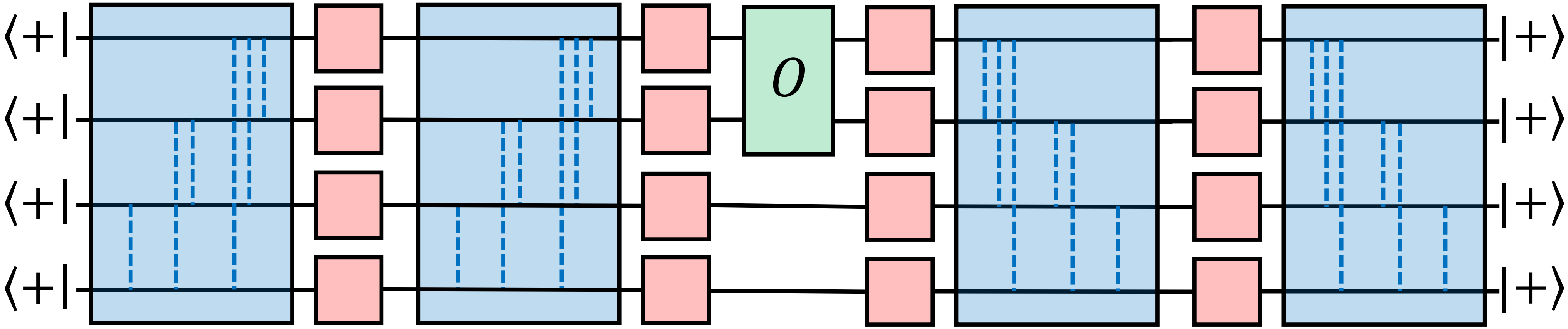
Quantum Mean Value problem for level-2 QAOA



B-layers: single-qubit X-rotations

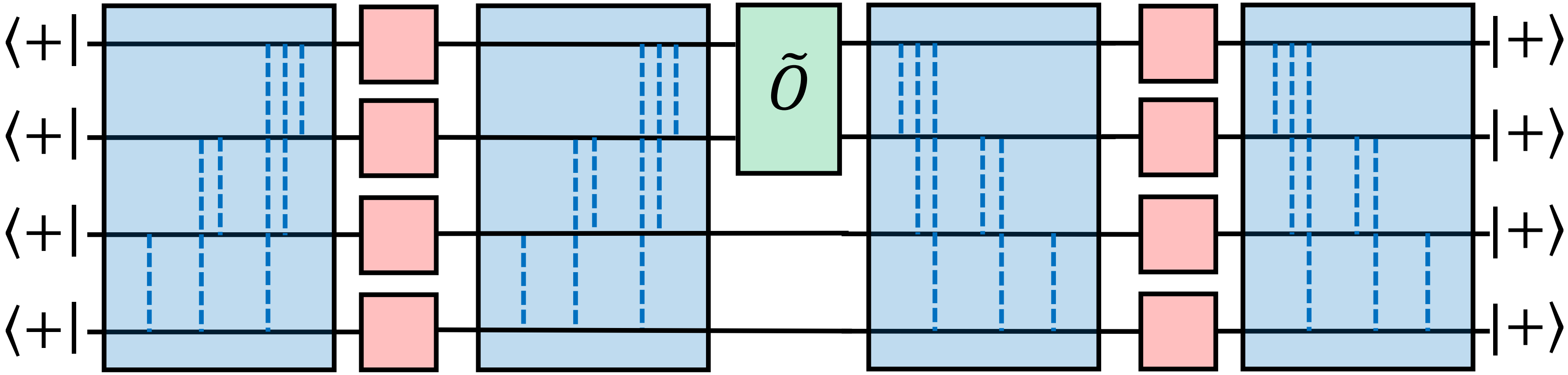
C-layers: diagonal two-qubit gates

Quantum Mean Value problem for level-2 QAOA



Step 1: conjugate the observable O by the inner B-layers.
This gives a modified two-qubit observable $\tilde{O}$.

Quantum Mean Value problem for level-2 QAOA



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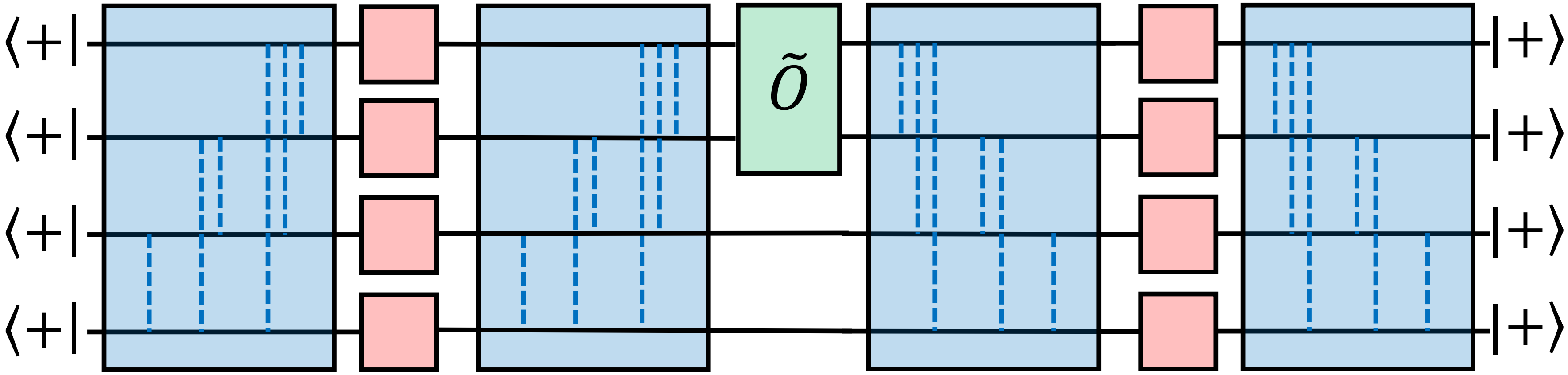
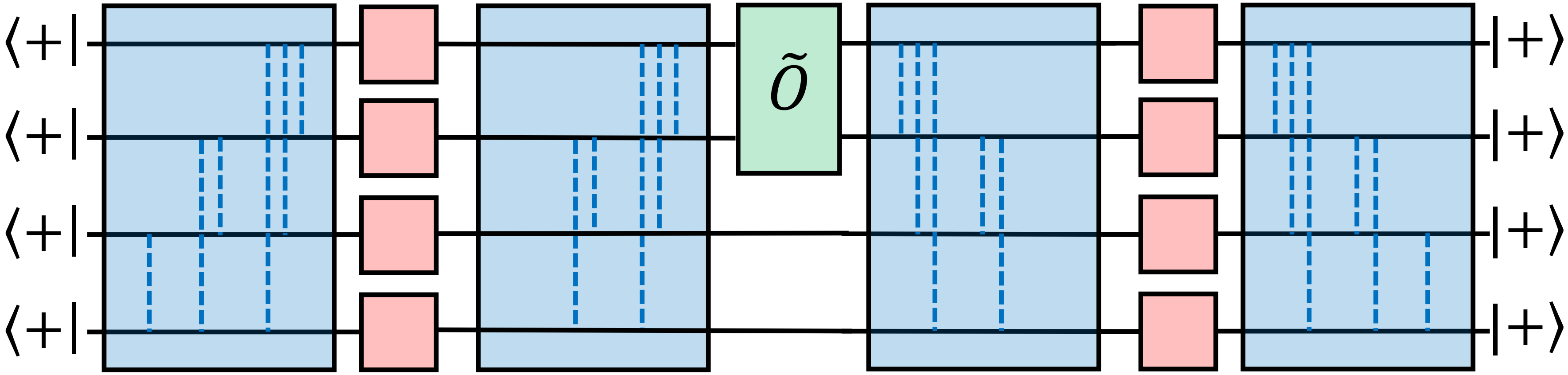


Step 2: conjugate $\tilde{O}$ by the inner C-layers

Quantum Mean Value problem for level-2 QAOA



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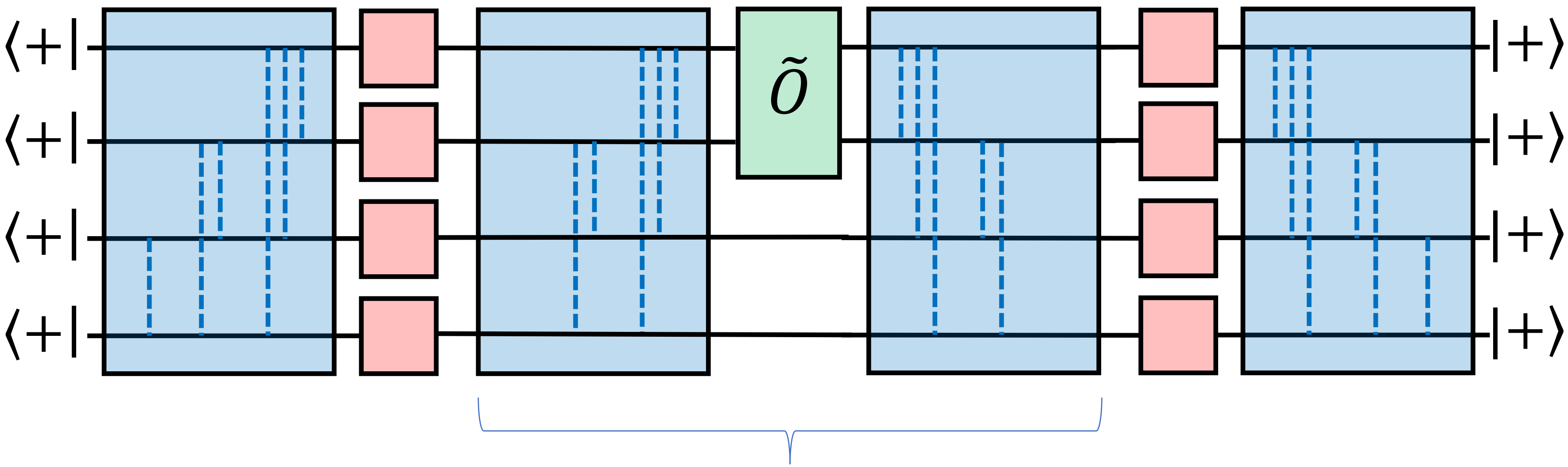
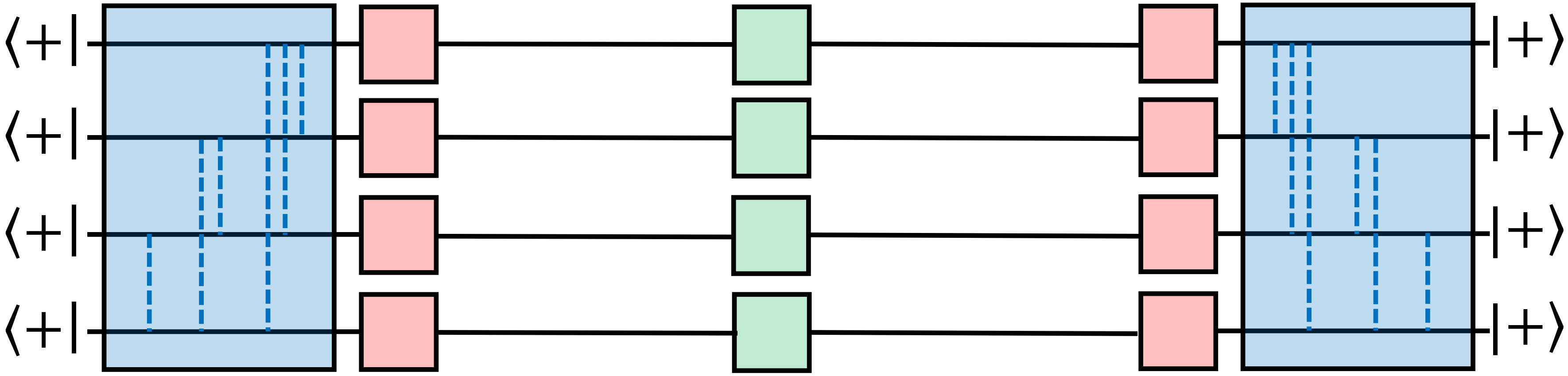
Quantum Mean Value problem for level-2 QAOA



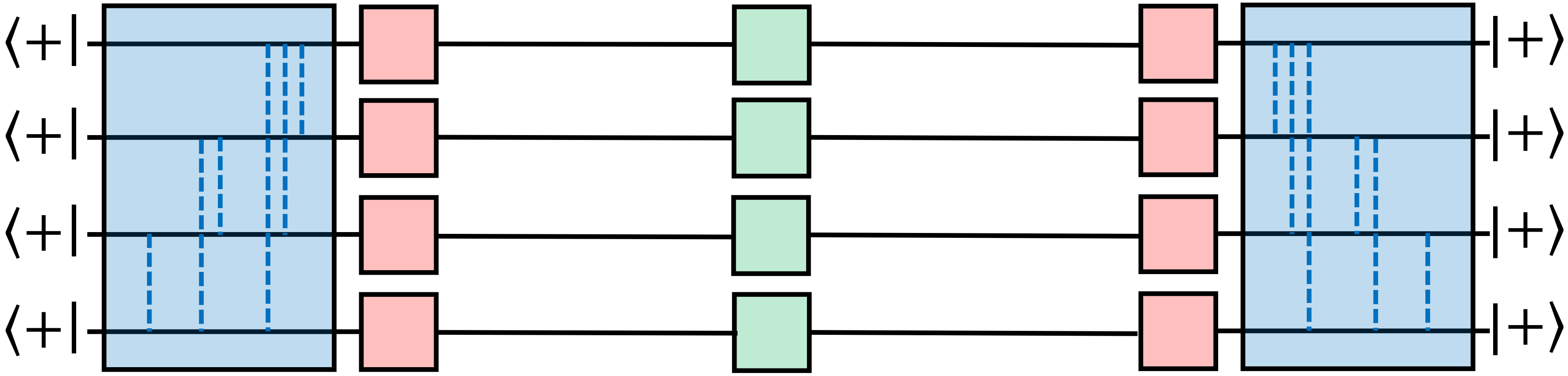
Linear combination of $O(1)$
tensor product observables

Quantum Mean Value problem for level-2 QAOA



$$P = P_1 \otimes P_1 \otimes \cdots \otimes P_n$$

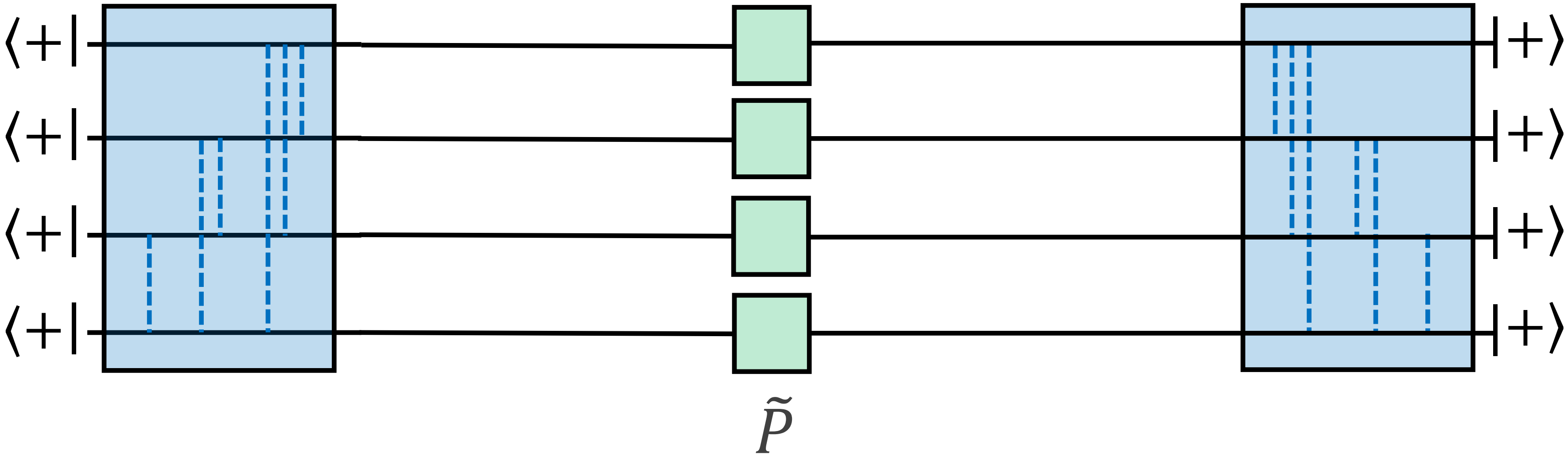
Quantum Mean Value problem for level-2 QAOA



$$P = P_1 \otimes P_1 \otimes \cdots \otimes P_n$$

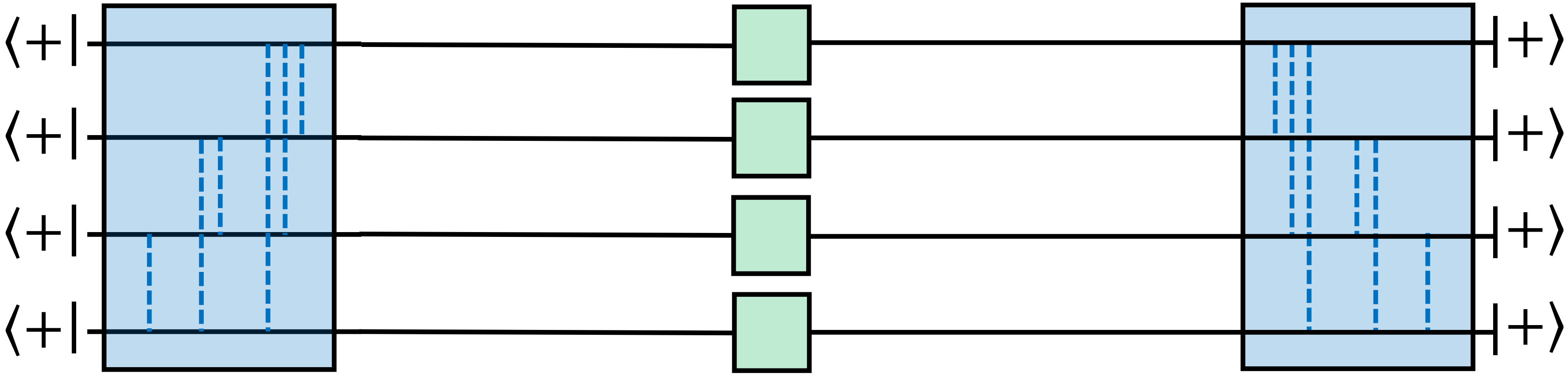
Step 3: conjugate the observable P by the inner B-layers.

Quantum Mean Value problem for level-2 QAOA



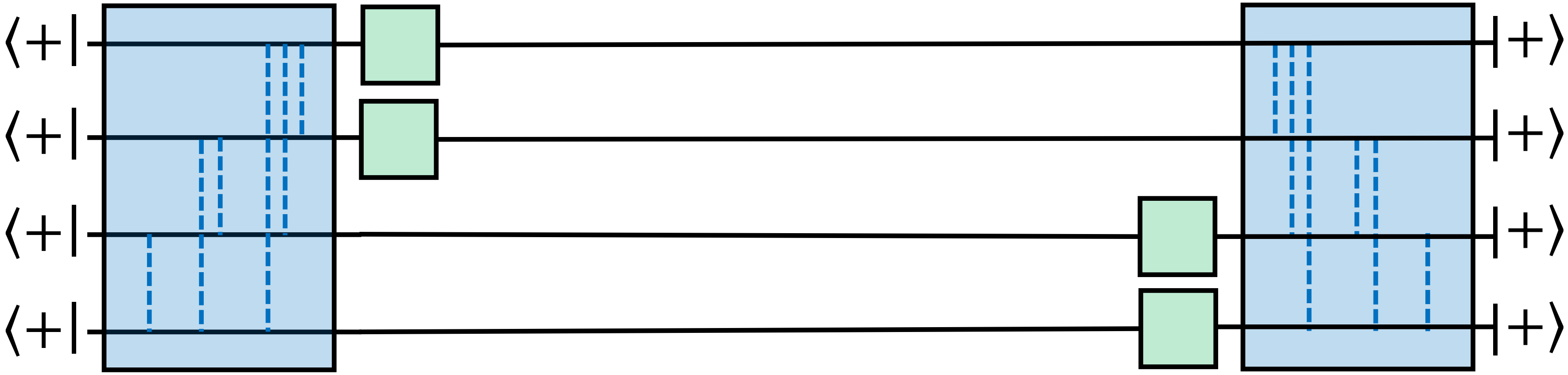
Step 3: conjugate the observable P by the inner B-layers.
This gives a modified tensor product observable $\tilde{P}$.

Quantum Mean Value problem for level-2 QAOA



Step 4: express the QMV as the inner product of computationally tractable states.

Quantum Mean Value problem for level-2 QAOA



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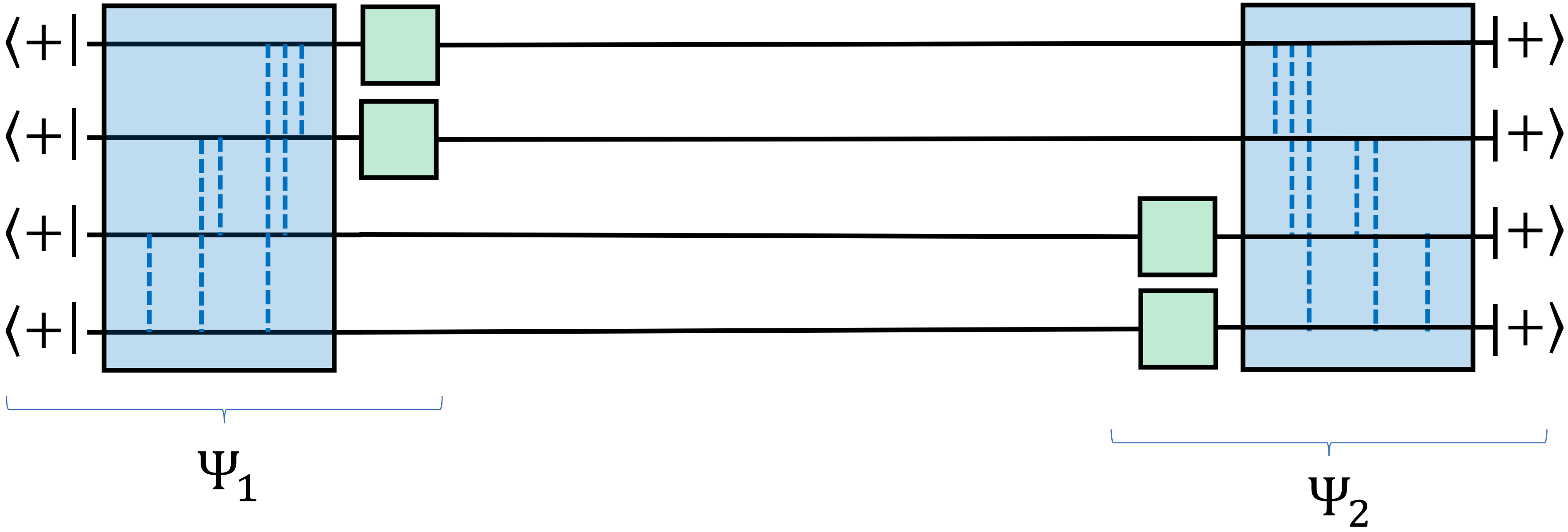

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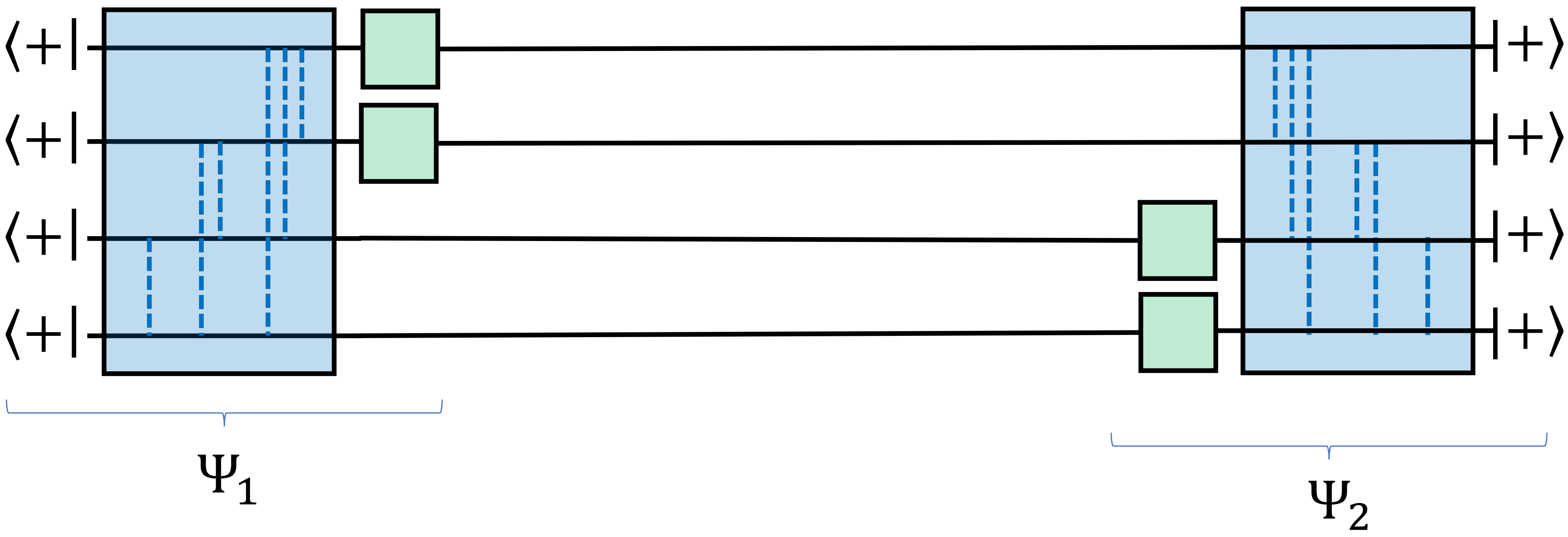
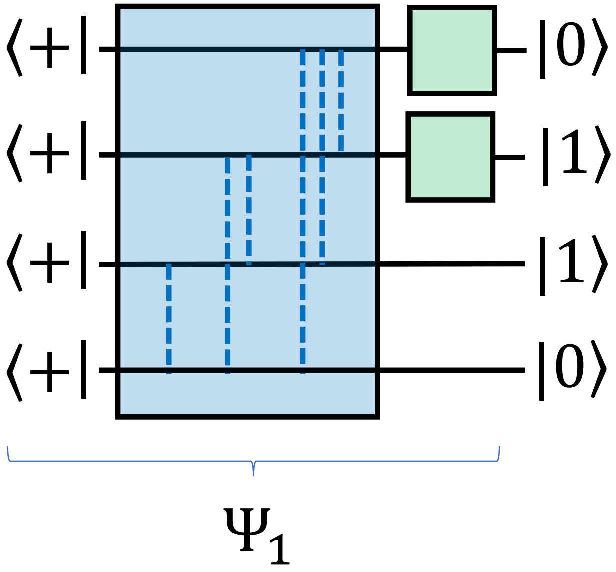
Quantum Mean Value problem for level-2 QAOA



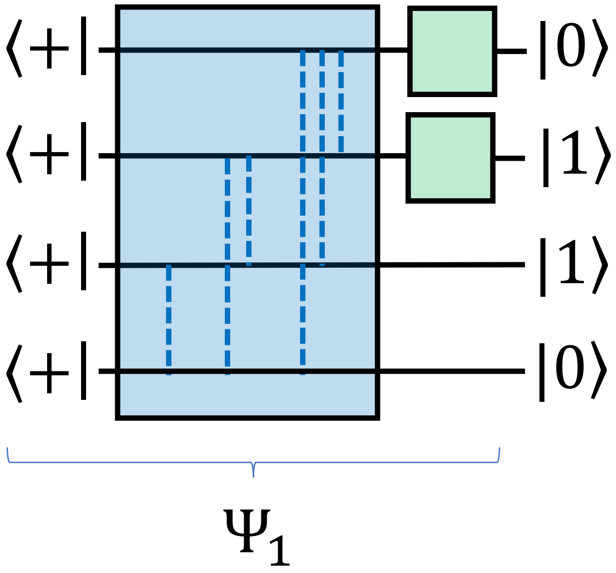
Step 4: express the QMV as the inner product of computationally tractable states. Approximate the inner product $\langle\Psi_1|\Psi_2\rangle$ using Van den Nest algorithm.

Quantum Mean Value problem for level-2 QAOA



Claim:
any amplitude $\langle \Psi_1 | x \rangle$ can be computed in time roughly $2^{n/2}$.

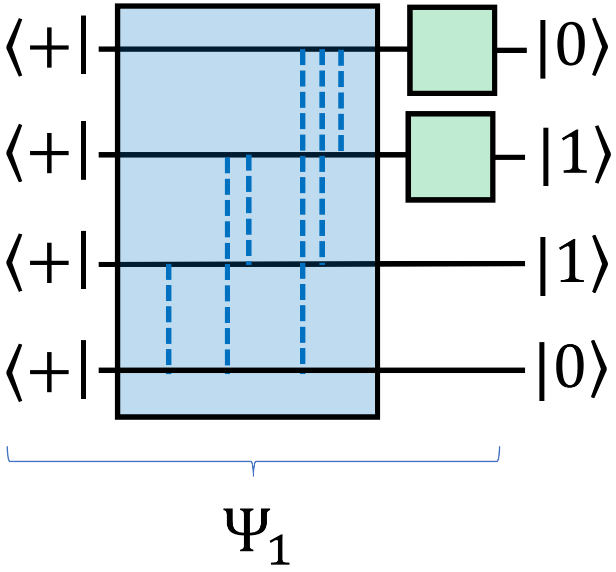
Quantum Mean Value problem for level-2 QAOA



Claim:
any amplitude $\langle\Psi_1|x\rangle$ can be computed in time roughly $2^{n/2}$.

- The C-layer includes only diagonal two-qubit gates
- It cannot entangle a qubit initialized in a basis state
- Half of all qubits remains unentangled

Quantum Mean Value problem for level-2 QAOA



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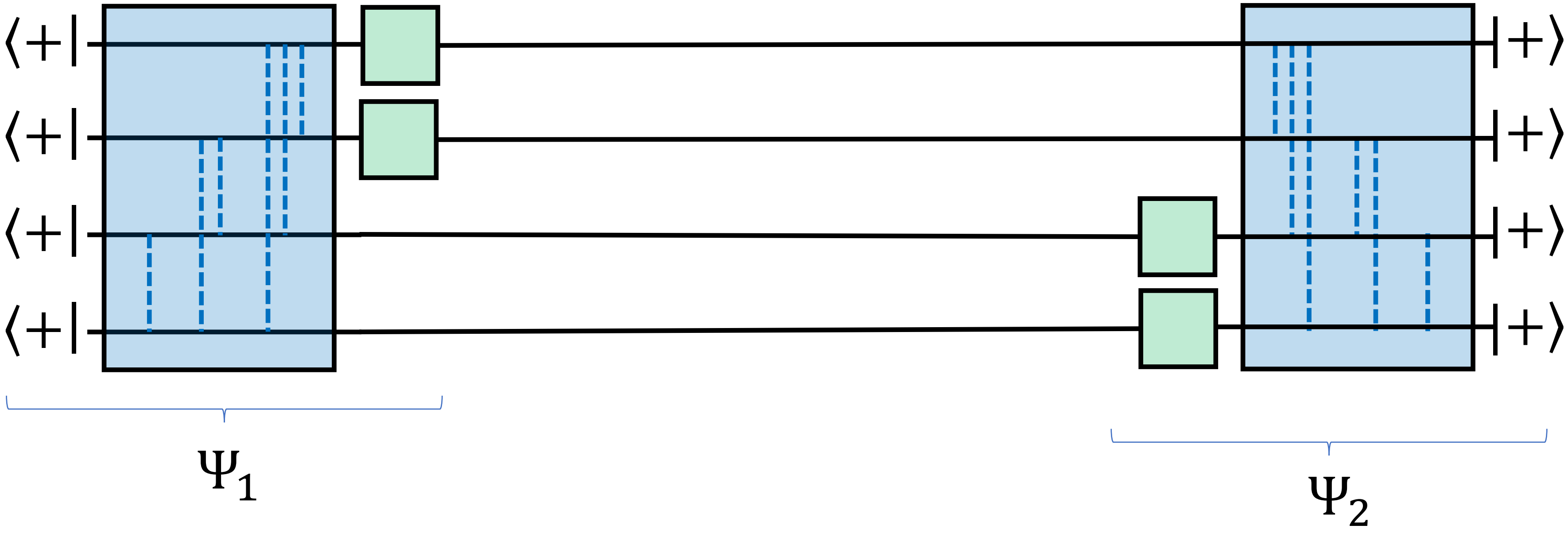
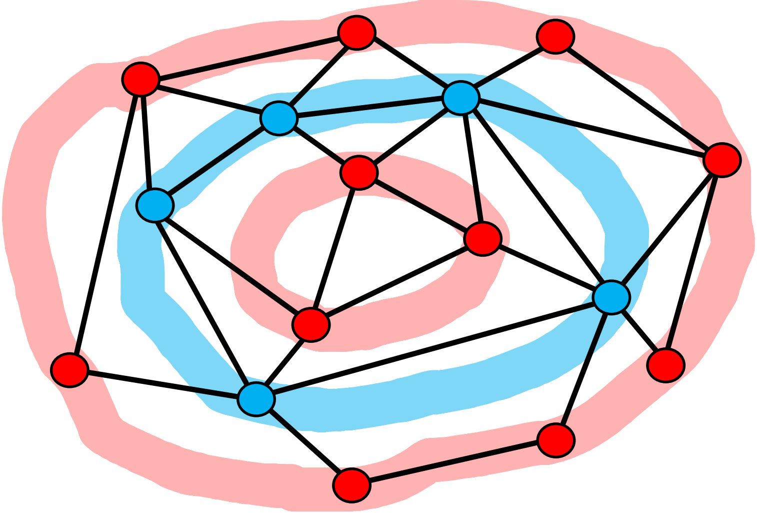
Approximating the inner product $\mathrm{QMV} = \langle \Psi_1 | \Psi_2 \rangle$ by Monte-Carlo takes time $2^{n/2} \epsilon^{-2}$

Quantum Mean Value problem for level-2 QAOA



Suppose the C-layer only includes nearest-neighbor gates on a planar graph.
Can we pick a good partition of qubits making Ψ_1 and Ψ_2 less entangled ?

Theorem. Suppose $G = (V, E)$ is a planar graph. There exists a partition $V = V_1 V_2$ such that the subgraphs of G induced by V_1 and V_2 have treewidth at most 2. Such partition can be efficiently computed.



DeVos et al, "Excluding any graph as a minor allows a low tree-width 2-coloring" (2004)

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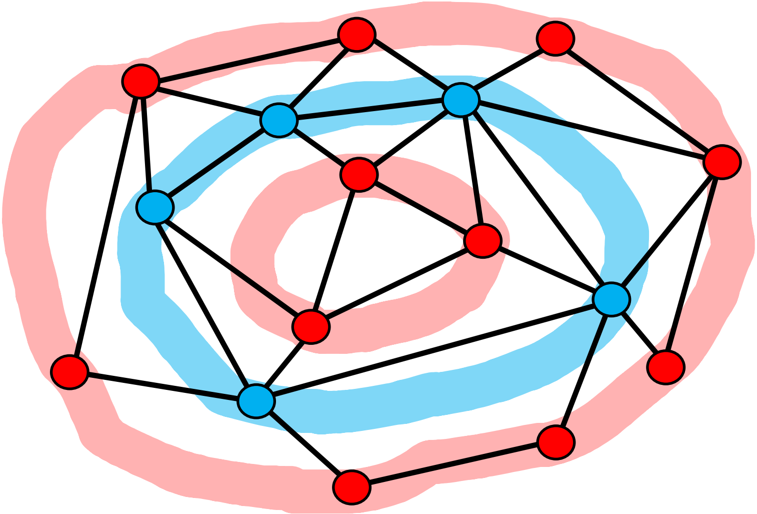

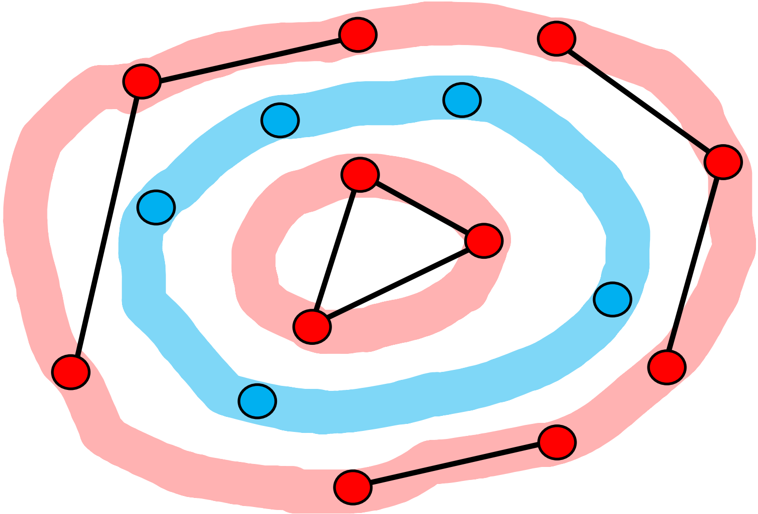

Subgraph induced by V_1

DeVos et al, "Excluding any graph as a minor allows a low tree-width 2-coloring" (2004)

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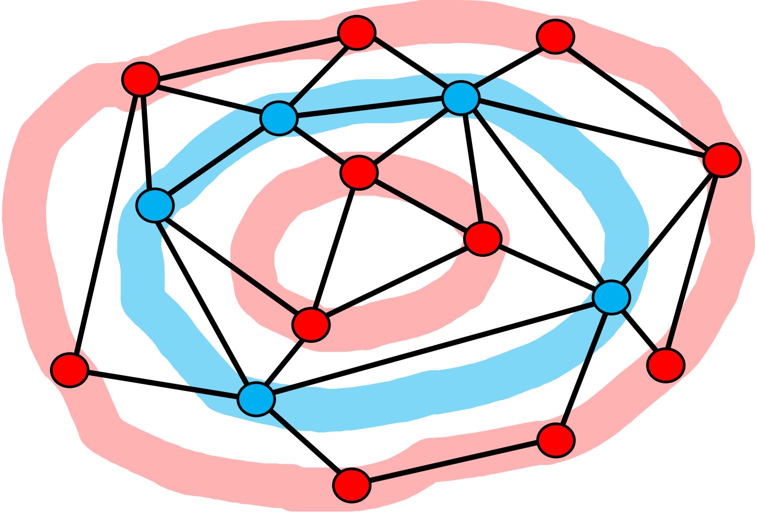
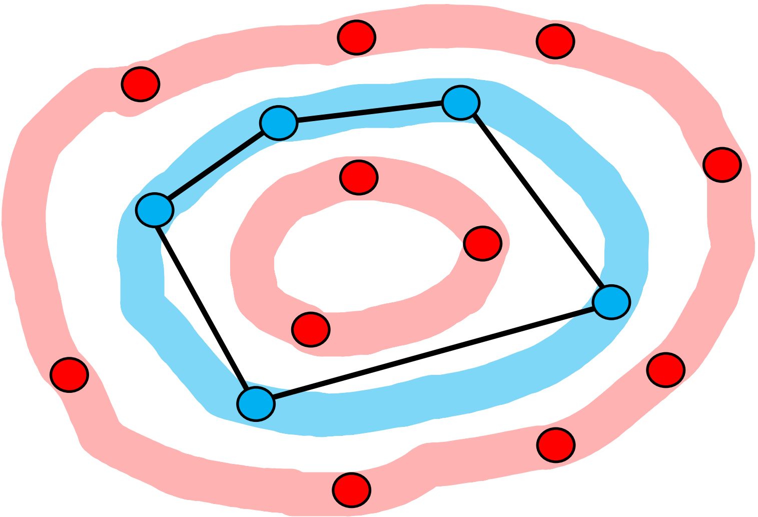
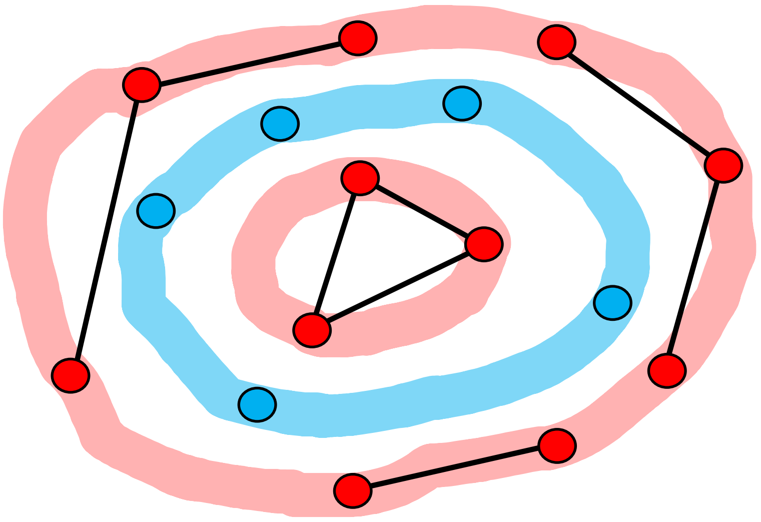


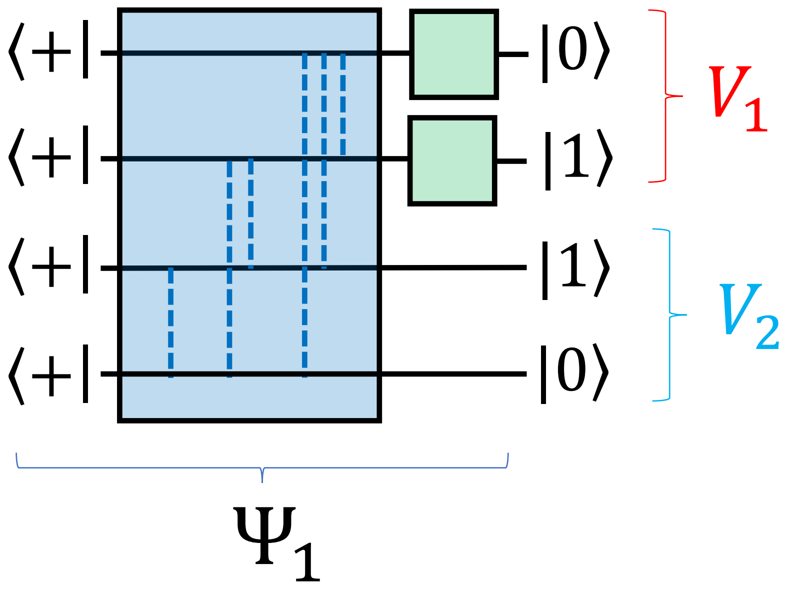


Subgraph induced by V_2

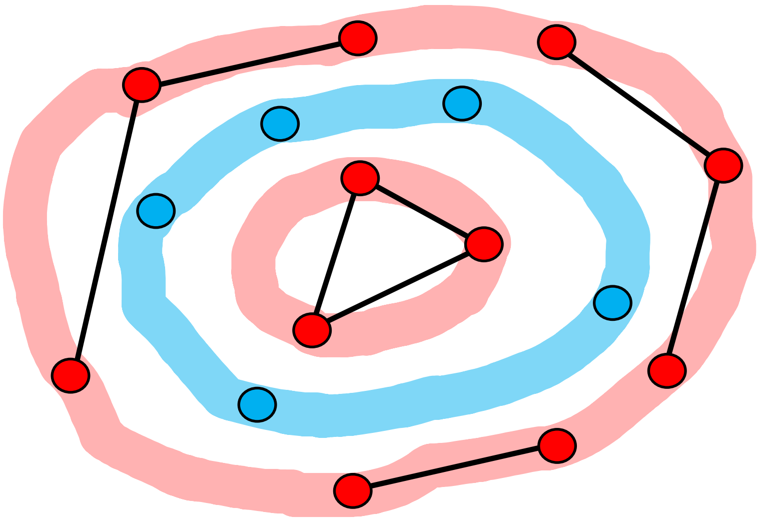
DeVos et al, "Excluding any graph as a minor allows a low tree-width 2-coloring" (2004)



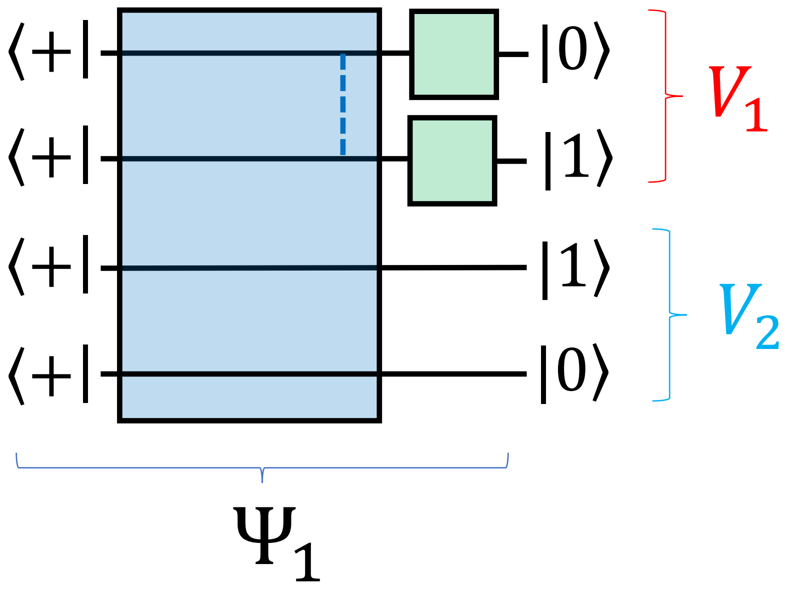
Subgraph induced by V_1



Two-qubit gates touching a qubit in V_2 disappear.



Subgraph induced by V_1



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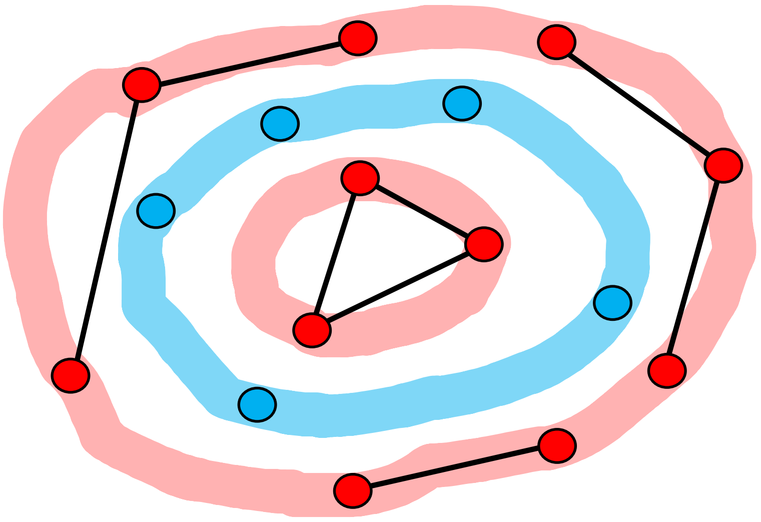

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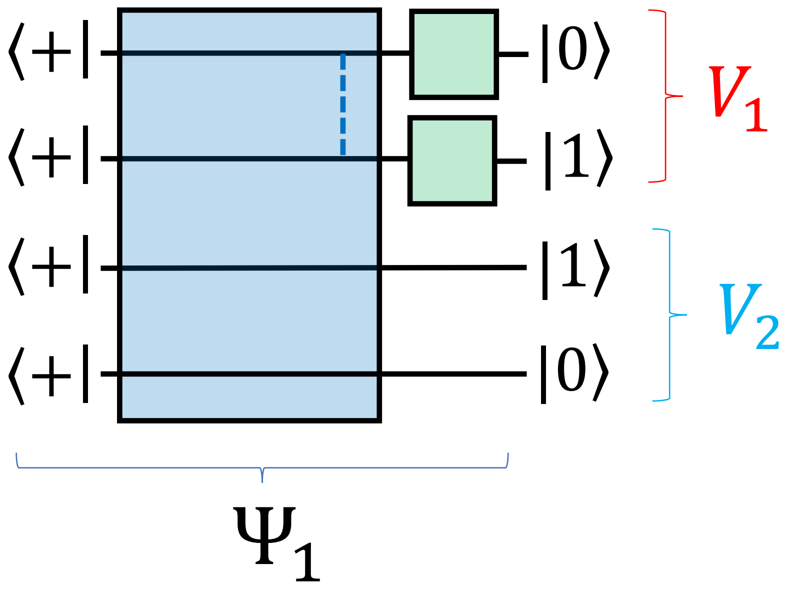

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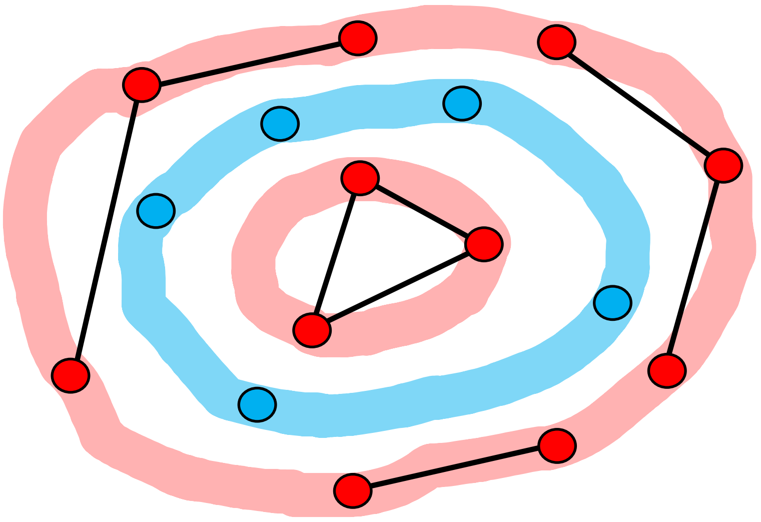
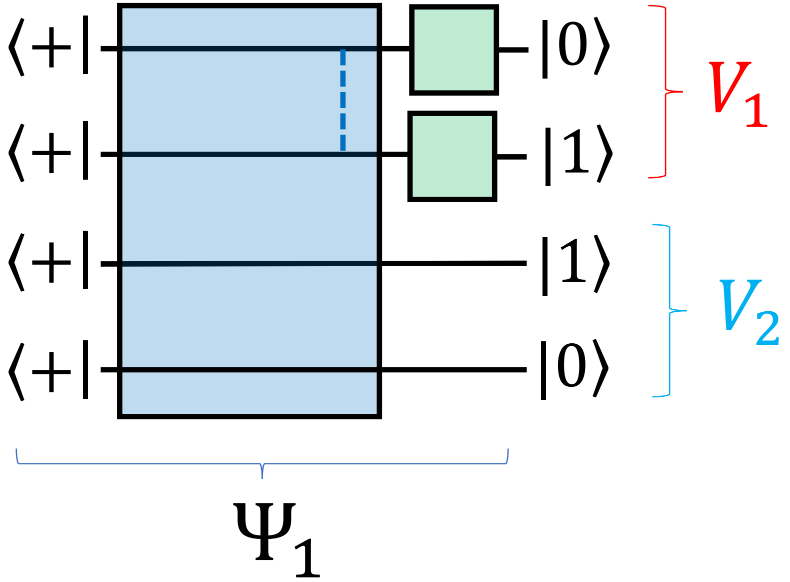
Amplitudes of Ψ_1 are defined by a tensor network on the subgraph induces by V_1.



Subgraph induced by V_1



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Amplitudes of Ψ_1 are defined by a tensor network on the subgraph induces by V_1.

Low-treewidth tensor networks are easy to contract. [Markov and Shi 2004]

Recap: we obtained a polynomial-time classical algorithm for approximating

$$\mathrm{QMV} = \langle \psi(\beta,\gamma) | Z_a Z_b | \psi(\beta,\gamma) \rangle$$

for level-2 QAOA states with the Ising-like cost function on any planar graph.

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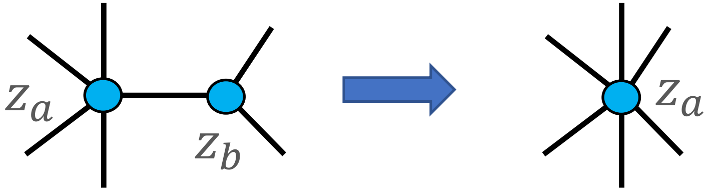
Bonus feature: RQAOA preserves planarity



variable elimination

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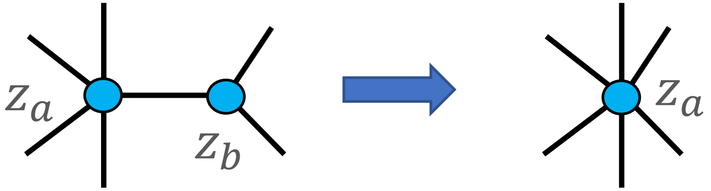

variable elimination

Corollary: level-2 RQAOA on planar graphs can be simulated classically in polynomial time.

Summary

- Variational quantum algorithms based on constant-depth geometrically local circuits in 2D can be simulated classically in linear time.

- Large-scale classical simulation of level-1 RQAOA is reported. Classical simulation of level-2 RQAOA is a work in progress.

Open problems

- Establish classical hardnes of approximating quantum mean values for low-depth circuits or low-level QAOA

- Rigorous bounds on the performance of RQAOA. More general variable elimination methods.