Imaginary Hamiltonian variational ansatz(iHVA) for QED and combinatorial optimization problems

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collaborate with

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Based on [arXiv:2408.09083]

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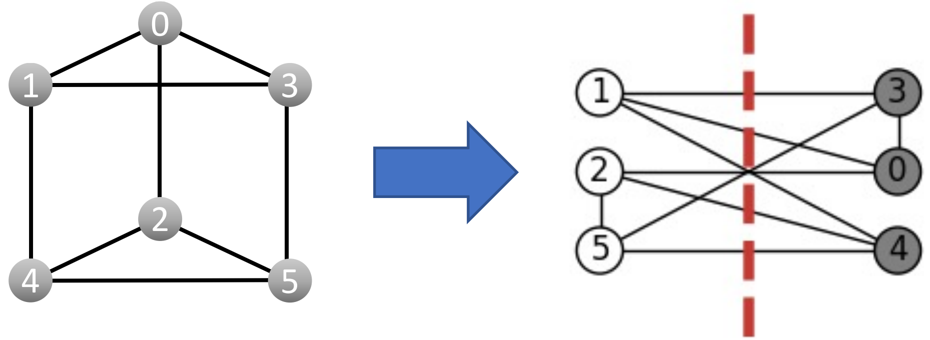
Main Content

- ❑ QAOA ansatz and its challenges
- ❑ imaginary Hamiltonian variational ansatz
- ❑ iHVA-tree and its performance on MaxCut
- ❑ Conclusion and outlooks

QAOA ansatz for MaxCut

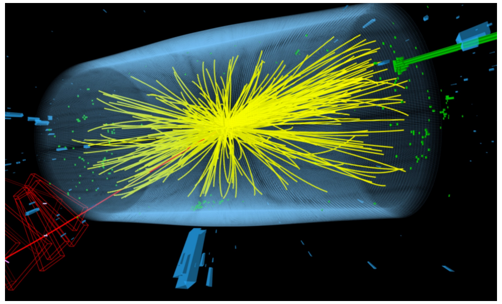
- **MaxCut:** Given an arbitrary graph with N nodes. Find a way to cut the maximum number of edges of the graph.



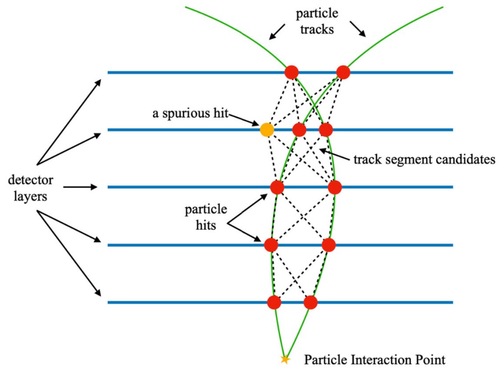
3-regular graph with number of nodes $N = 6$

[D-regular graph: every node connect with D edges.]

- **Applications:**



particle classification



track reconstruction

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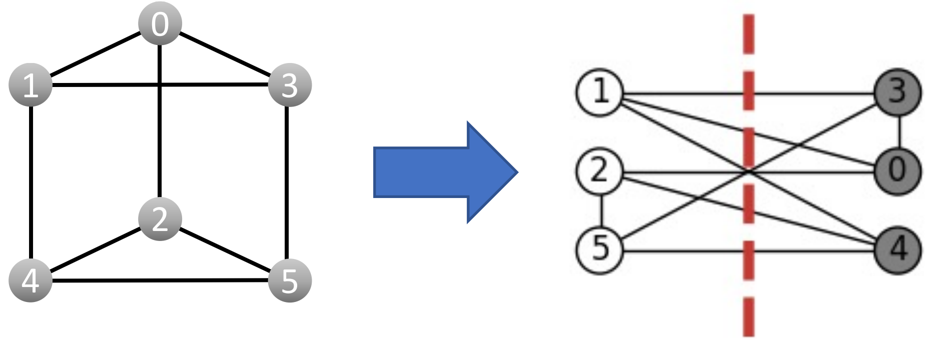

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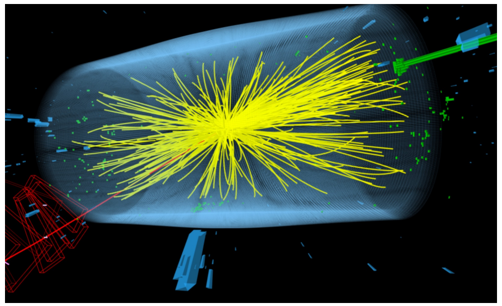

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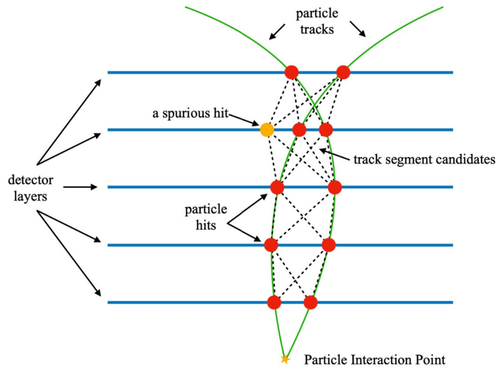

track reconstruction

Karp's 21 NP-complete problems [R. M. Karp, 1972]

- Satisfiability
  - 0-1 integer programming
  - Clique
    - Set packing
    - Vertex cover
      - Set cover
      - Feedback node set
      - Feedback arc set
      - Directed Hamiltonian cycle
        - Undirected Hamiltonian cycle
- 3-SAT
  - Chromatic number
    - Clique cover
    - Exact cover
      - Hitting set
      - Steiner tree
      - 3-d matching
      - Knapsack
        - Job sequencing
        - Partition
          - **MaxCut**

(MaxCut on 3-regular graphs is still NP-complete)

QAOA ansatz for MaxCut

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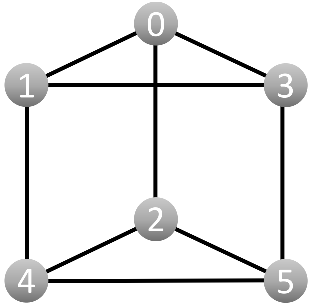
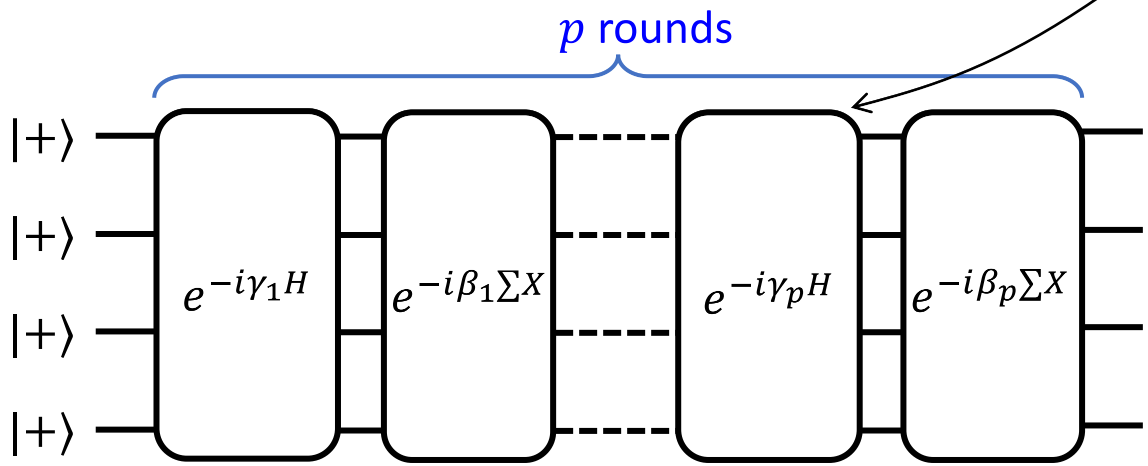


Ground state preparation of

$$H_{\mathrm{MC}} = \sum_{\langle i,j\rangle\in\mathcal{E}} (Z_i Z_j - 1)/2$$

$$e^{-iH_{\mathrm{MC}}t}$$

- **QAOA ansatz**(or Hamiltonian Variational Ansatz (HVA)):



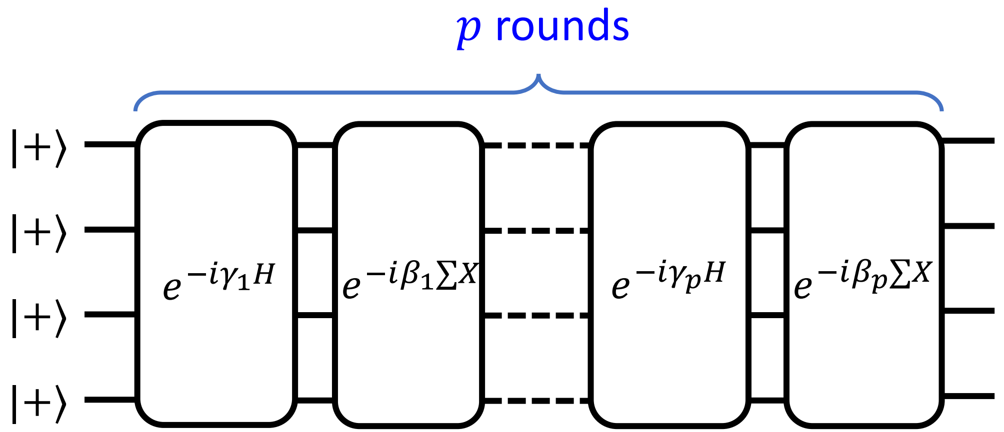
- Optimize γ and β until convergence. (See **Xingyu Guo** and **Enrico Rinaldi's** talk on Monday and Tuesday)
- Retrieve adiabatic evolution as $p \to \infty$

Challenges to QAOA

- Evaluate MaxCut performance of an algorithm

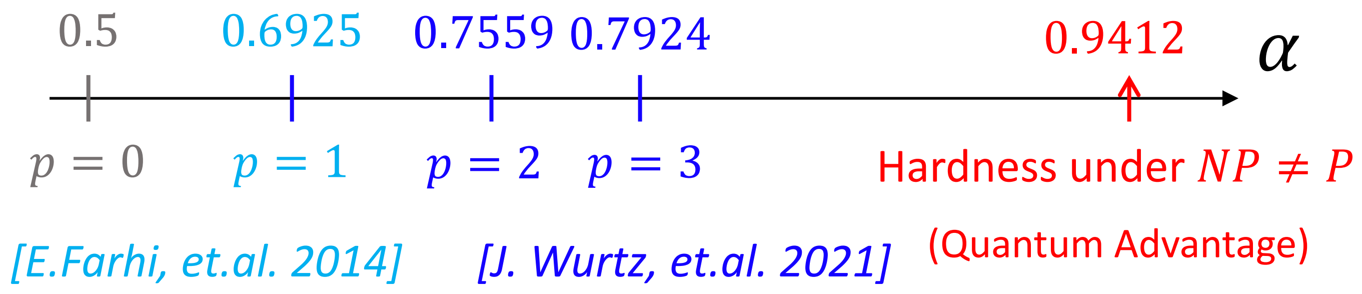
$$\alpha = \frac{\mathrm{cut}(x^*)}{\max_x \mathrm{cut}(x)} \in [0,1]$$

$$\mathrm{cut}(x^*) = -\min_{\boldsymbol{\gamma},\boldsymbol{\beta}} \langle \psi(\boldsymbol{\gamma},\boldsymbol{\beta}) | H_{\mathrm{MC}} | \psi(\boldsymbol{\gamma},\boldsymbol{\beta}) \rangle$$



- $p = \mathrm{const}$:No theoretical guarantees to surpass the classical algorithms *[B. Barak et. al. 2022]*。

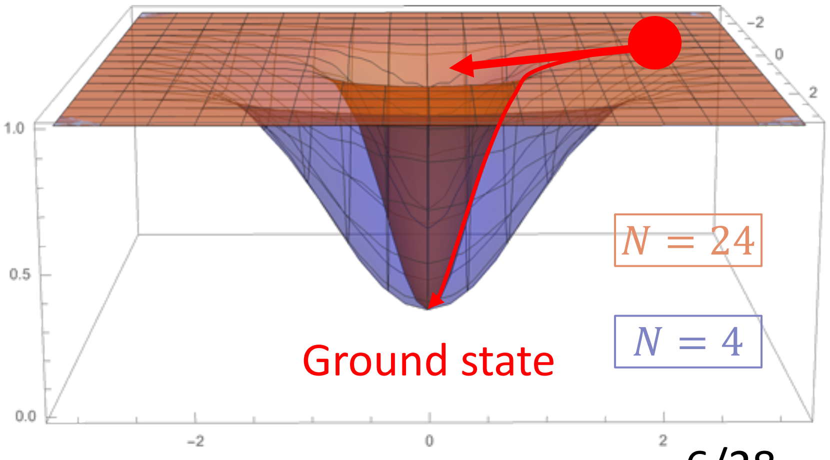
[For 3-regular graph]



- $p \propto N$: Barren Plateaus(BP) exist. The optimization is hard to perform*[McClean, et. al. 2018].*

vanishing gradient

$$\left\| \frac{\partial C(\boldsymbol{\theta})}{\partial \theta_i} \right\| \propto \frac{1}{2^N}$$

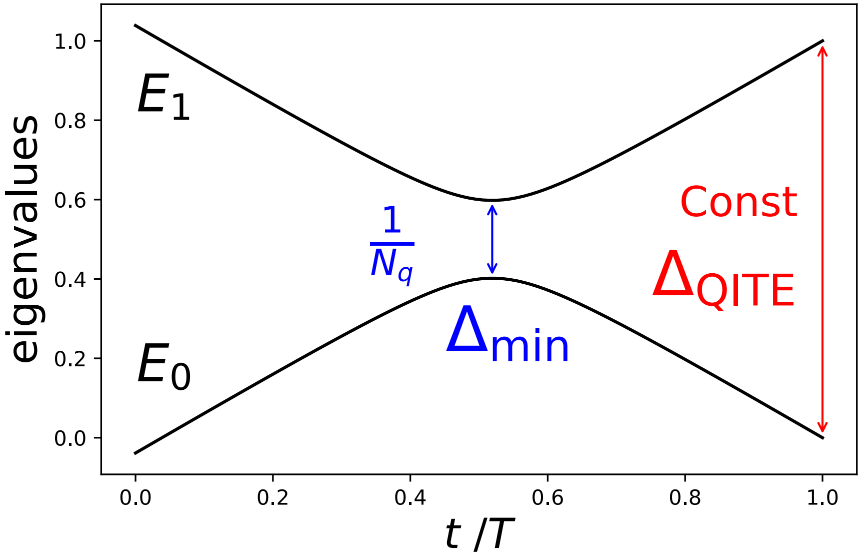


Challenges to QAOA

- In contrast, imaginary time evolution requires *constant* time.

$$e^{-\mathrm{T}H}|\Omega\rangle \sim e^{-\mathrm{T}\Delta_{\mathrm{QITE}}}|E_1\rangle + |E_0\rangle$$

$$\mathrm{T}_{\mathrm{Imag}} \propto \Delta_{\mathrm{QITE}}^{-1} = \mathrm{Const}$$



$$p \sim T_{\mathrm{Real}} \propto \Delta_{\min}^{-1} \propto N$$

- $p = \mathrm{const}$:No theoretical guarantees to surpass the classical algorithms *[B. Barak et. al. 2022]*。

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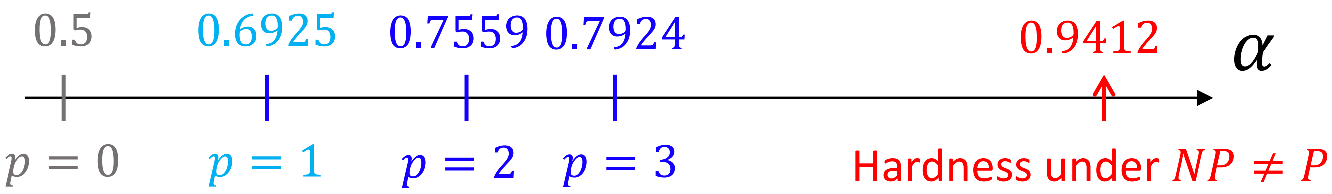

[E.Farhi, et.al. 2014] *[J. Wurtz, et.al. 2021]* (Quantum Advantage)

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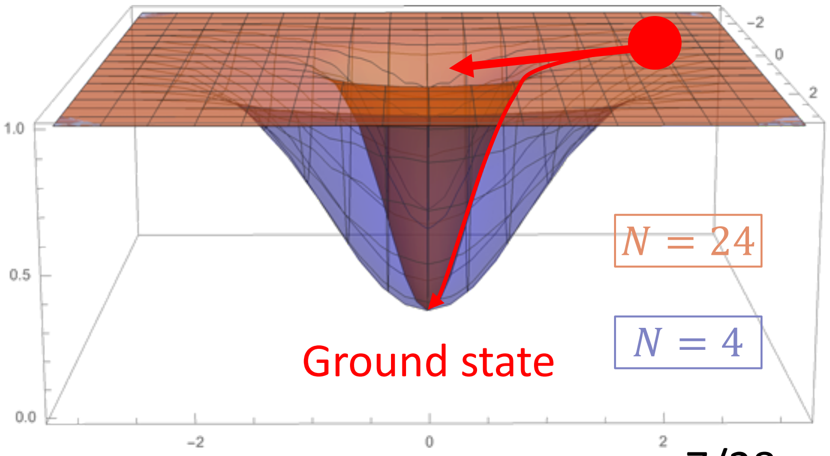

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imaginary time evolution by unitary quantum gates

Consider the following Hamiltonian

$$H_1 \equiv -Z = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

The initial state of the evolution is

$$|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

The imaginary time evolution of the state is

$$e^{-\tau H_1}|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{\tau} & 0 \\ 0 & e^{-\tau} \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \propto \frac{1}{\sqrt{e^{2\tau} + e^{-2\tau}}}\begin{pmatrix} e^{\tau} \\ e^{-\tau} \end{pmatrix}$$

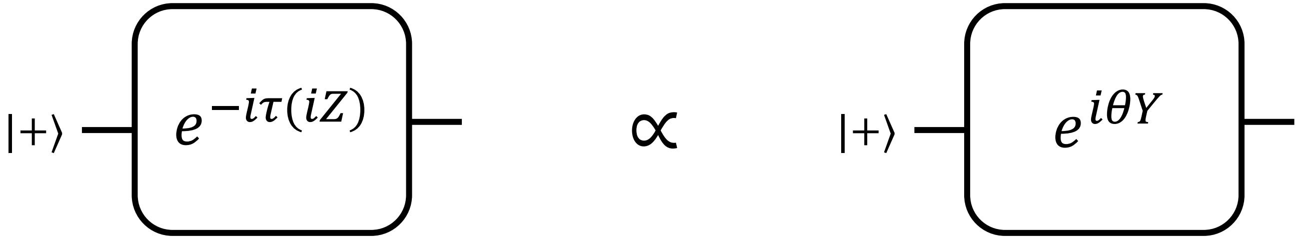
The evolution can be realized by a single-qubit R_Y rotation

$$e^{i\theta Y}|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \cos\theta + \sin\theta \\ \cos\theta - \sin\theta \end{pmatrix}$$

$$e^{\tau Z}|+\rangle \propto e^{i\theta(\tau)Y}|+\rangle$$

[M. Motta et al. Nat. Phys. (2020)]

imaginary time evolution by unitary quantum gates



imaginary Hamiltonian Variational Ansatz (iHVA)

imaginary time evolution of Z → real time evolution of Y

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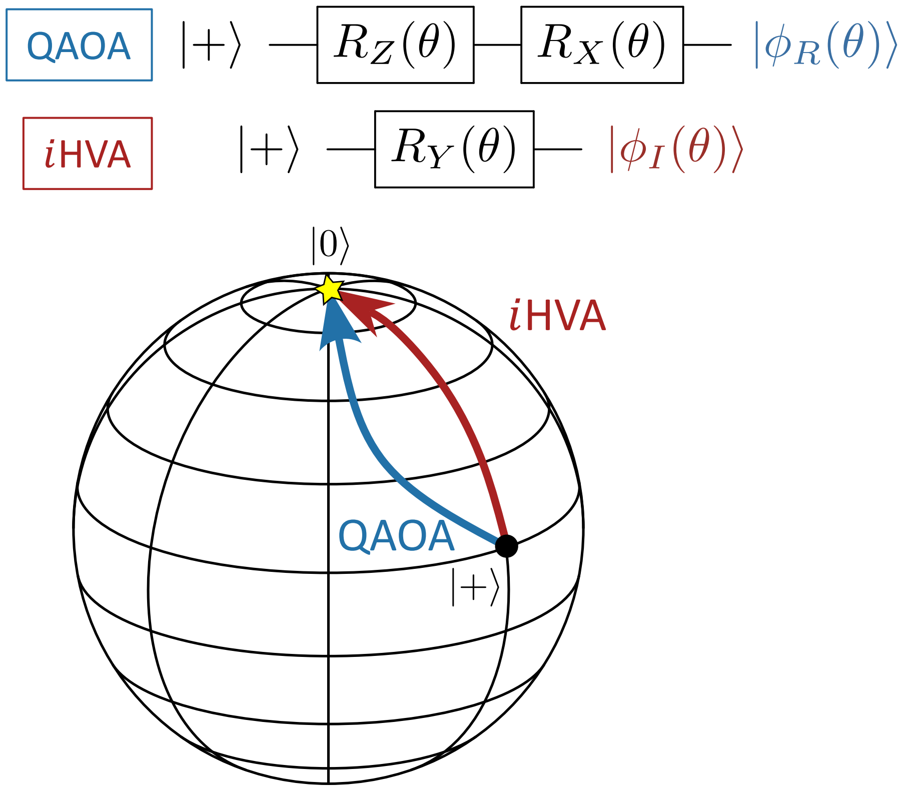
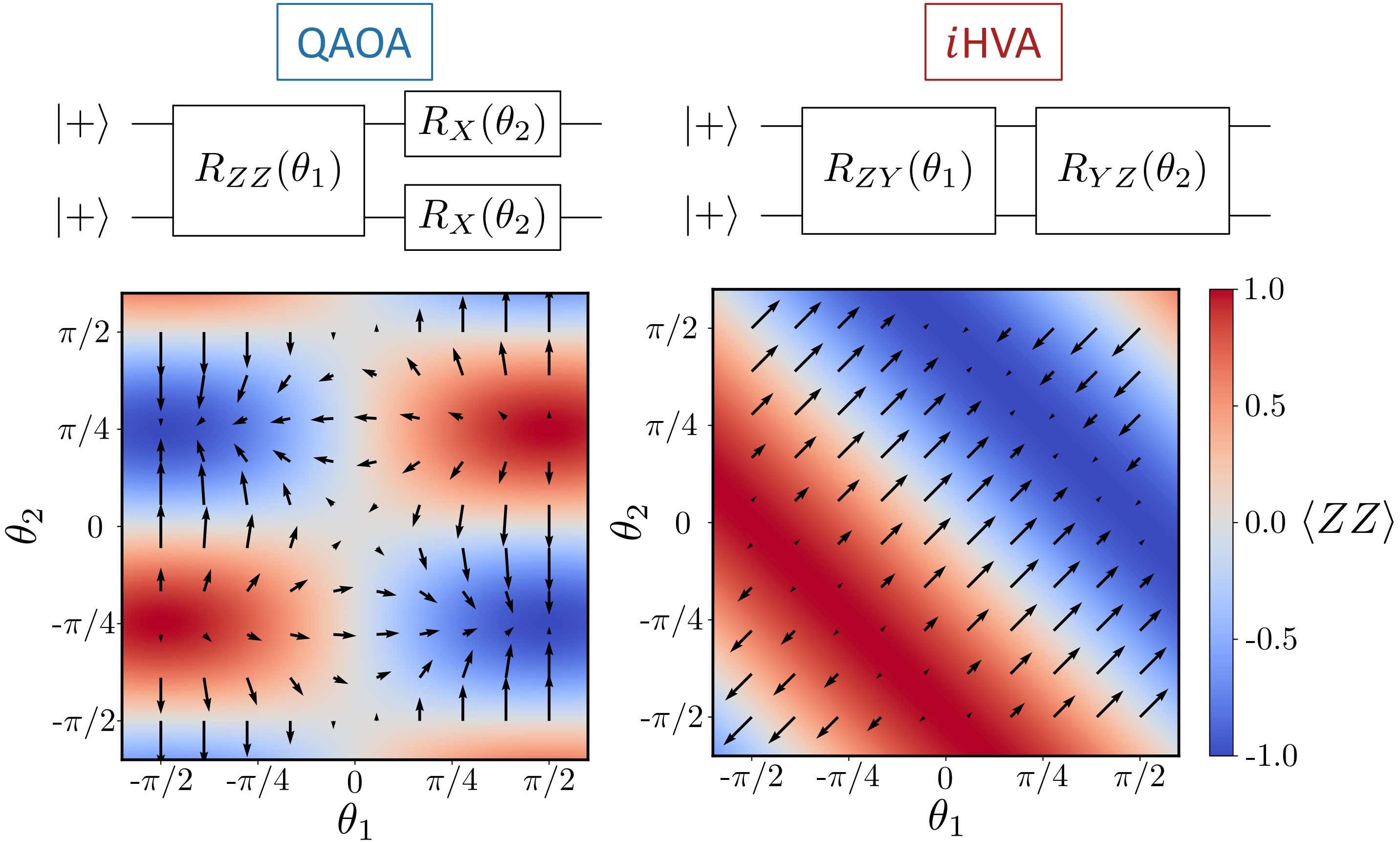
imaginary Hamiltonian Variational Ansatz on toy models

- To prepare the ground state of $H_1 = -Z$.



- The variational optimization path on Bloch sphere. The iHVA path is geodesic. Its optimization steps is **less** than QAOA.

- To prepare the ground state of $H_2 = ZZ$.



- The energy landscape of two ansätze. The landscape of QAOA has a saddle point, which challenges the optimization. While iHVA does not have this problem.

iHVA for arbitrary quantum systems

- Consider a local interacting Hamiltonian

$$H = \sum_{\mu} H_{\mu}$$

- The imaginary time evolution is expanded by

$$e^{-\tau H_{\mu}} \propto \prod_{m \in \mathcal{P}_{\mathbb{S}_{\mu}}} e^{-i\theta_{\mu}^{(m)} \sigma_{\mu}^{(m)}}$$

$$\sigma_{\mu}^{(m)} \in \mathrm{span}\{\sigma \in \mathcal{P}_{\mathbb{S}_i}\}$$

- $\sigma_{\mu}^{(m)}$ derived by system symmetries

$$\left[U_g, \sigma_{\mu}^{(m)}\right] = 0 \qquad \left([U_g, H_{\mu}] = 0\right)$$

[**X. Wang**, Y. Chai, M. Demidik, X. Feng, K. Jansen, C. Tuysuz. arXiv:2307.13598]

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$$H_{\mathrm{MaxCut}} = \sum_{(i,j)\in\mathcal{E}} Z_i Z_j$$

$$\begin{aligned} e^{-\epsilon ZZ} \propto\ & e^{ia_1\epsilon II} \times e^{ia_2\epsilon IX} \times e^{ia_3\epsilon IY} \times e^{ia_4\epsilon IZ} \\ & \times e^{ia_5\epsilon XI} \times e^{ia_6\epsilon XX} \times e^{ia_7\epsilon XY} \times e^{ia_8\epsilon XZ} \\ & \times e^{ia_9\epsilon YI} \times e^{ia_{10}\epsilon YX} \times e^{ia_{11}\epsilon YY} \times e^{ia_{12}\epsilon YZ} \\ & \times e^{ia_{13}\epsilon ZI} \times e^{ia_{14}\epsilon ZX} \times e^{ia_{15}\epsilon ZY} \times e^{ia_{16}\epsilon ZZ} \end{aligned}$$

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: time-reversal symmetry $U_g = K$

: spin-flip symmetry $U_g = XX$

$$\sigma_{(i,j)}^{(1)} = Z_i Y_j \qquad \sigma_{(i,j)}^{(2)} = Y_i Z_j$$

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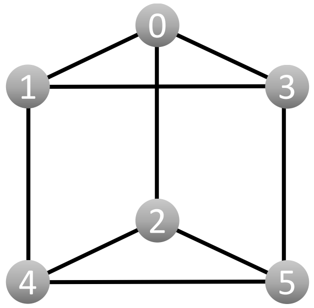
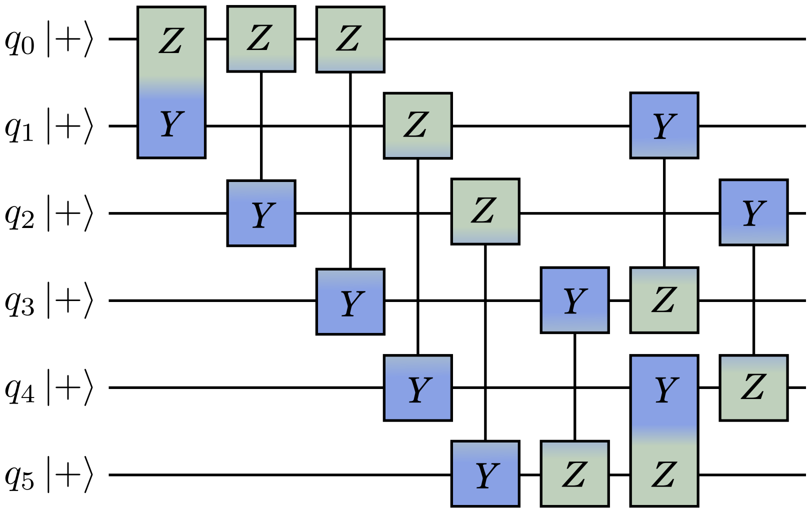


$$e^{-i\theta_{(i,j)} Z_i Y_j / 2}$$



$$\sigma_{(i,j)}^{(1)} = Z_i Y_j \qquad \sigma_{(i,j)}^{(2)} = Y_i Z_j$$

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iHVA of the Schwinger model

$$H_{\text{QED}} = \int \mathrm{d}x \left[-i\bar{\psi}\gamma^1(\partial_1 - igA_1)\psi + m\bar{\psi}\psi + \frac{1}{2}\left(\dot{A}_1 + l_0\right)^2 \right]$$

local $U(1)$ gauge invariance $\left[H_{\text{QED}}, \hat{G}_x\right] = 0,$

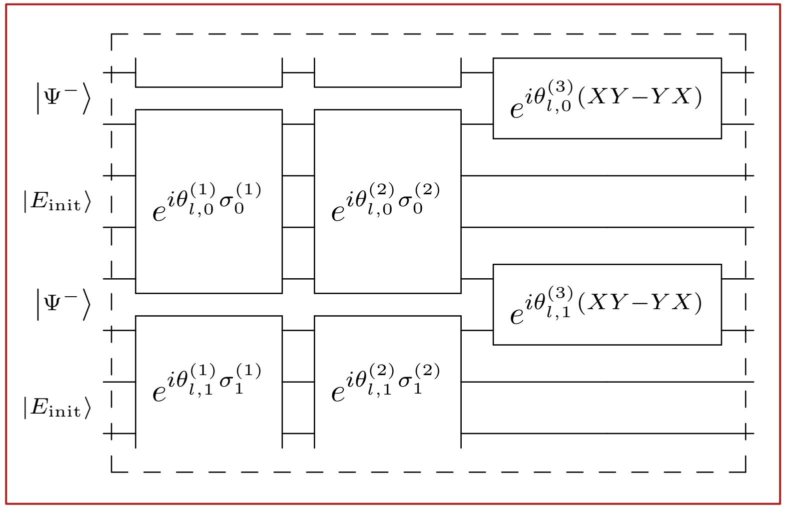
$$\hat{G}_x \equiv \hat{E}_x - \hat{E}_{x-1} - \hat{q}_x$$

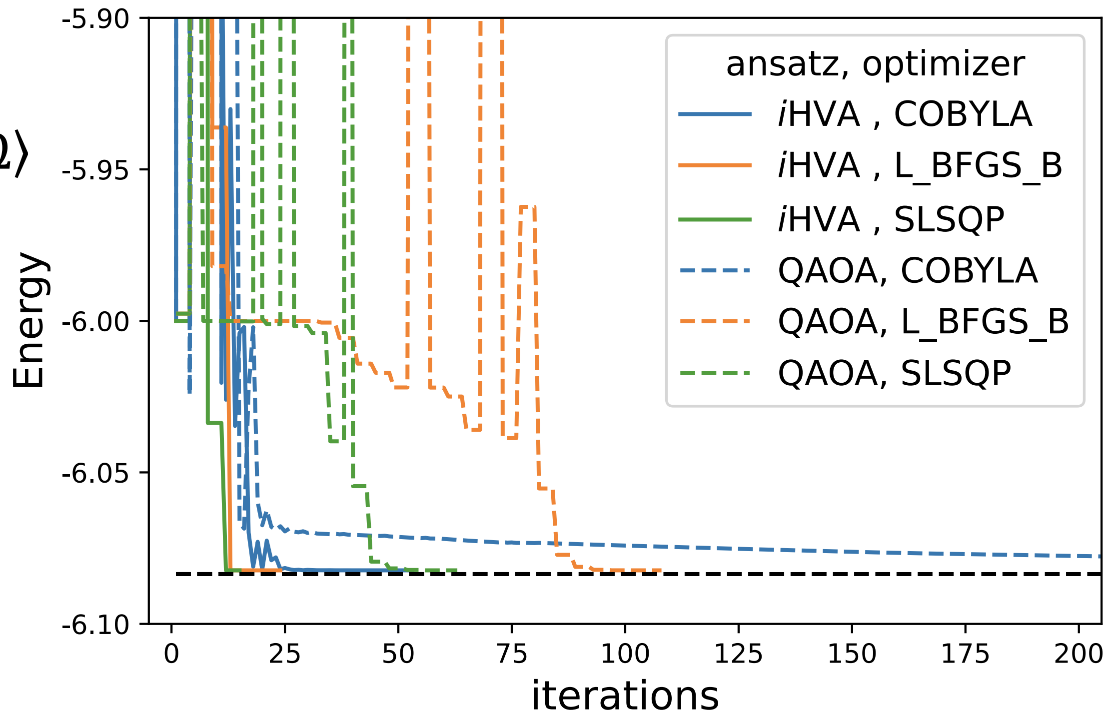
$$e^{-\tau(XX+YY)}|\Omega\rangle \propto e^{-i\theta(\tau)\,(XY-YX)}|\Omega\rangle$$

$$e^{-\tau(\psi_x^\dagger U_{x,x+1}\psi_{x+1}+h.c.)}|\Omega\rangle \propto e^{-i\theta(\tau) i(\psi_x^\dagger U_{x,x+1}\psi_{x+1}-h.c.)}|\Omega\rangle$$

UCC ansatz

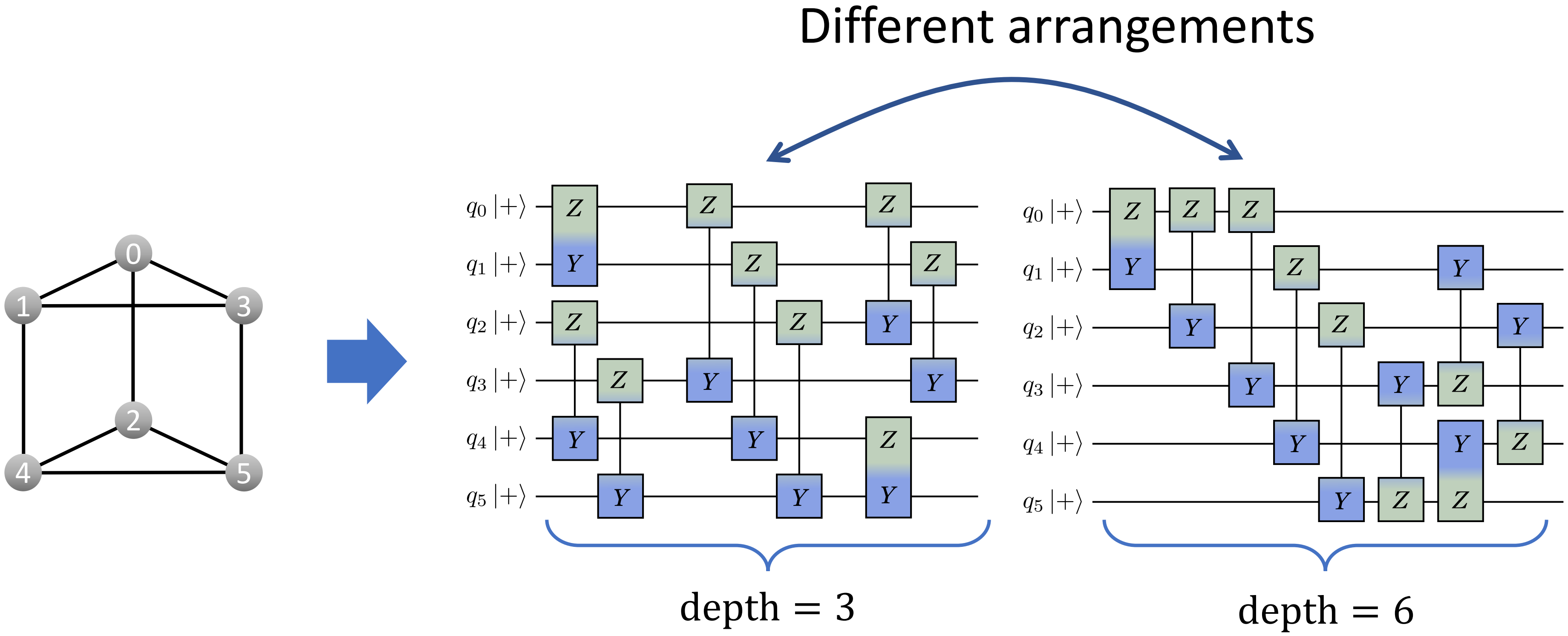
iHVA





- Ground state preparation of the Schwinger model using iHVA and QAOA. iHVA converges faster to the ground state than QAOA.

Different arrangements in iHVA



- Numerically, we find arrangement with larger depth gets more accurate results.

How to choose an appropriate arrangement?

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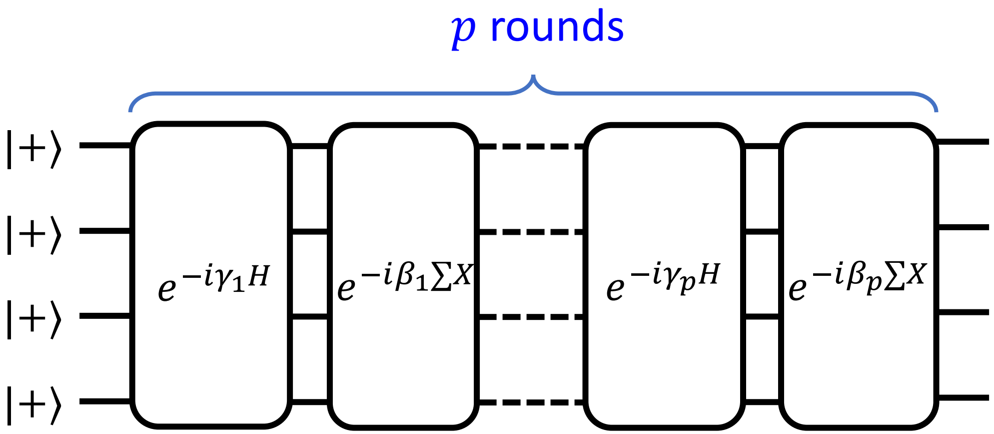
Challenges to QAOA



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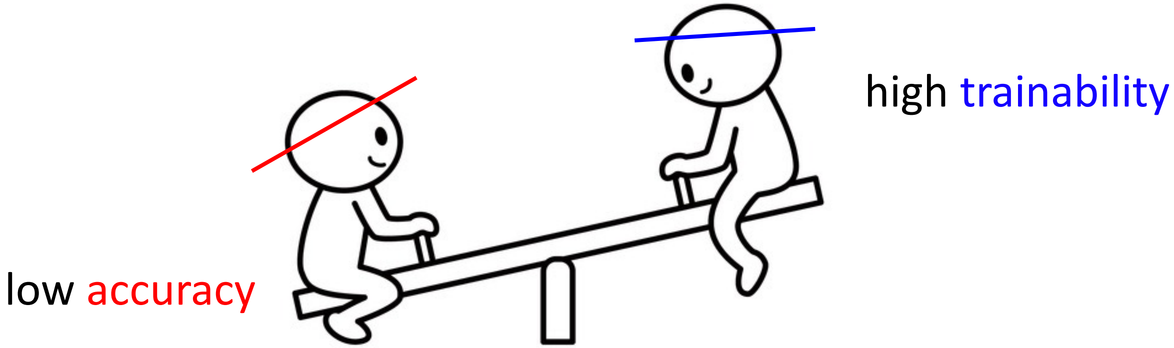
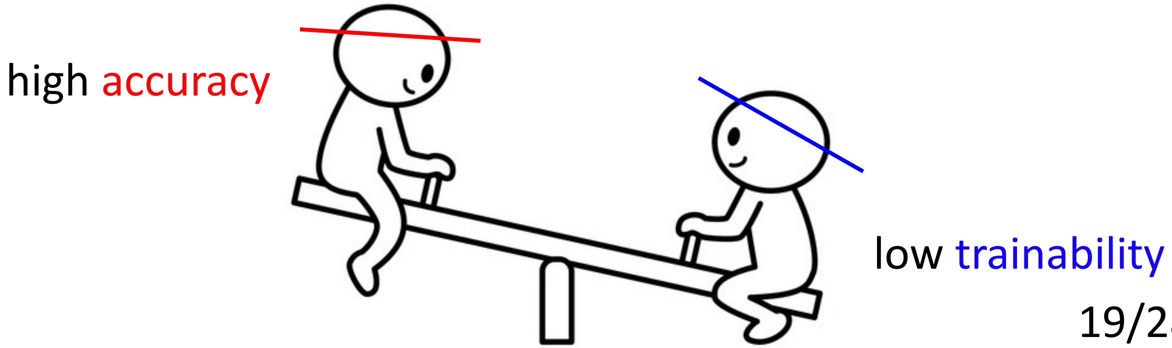


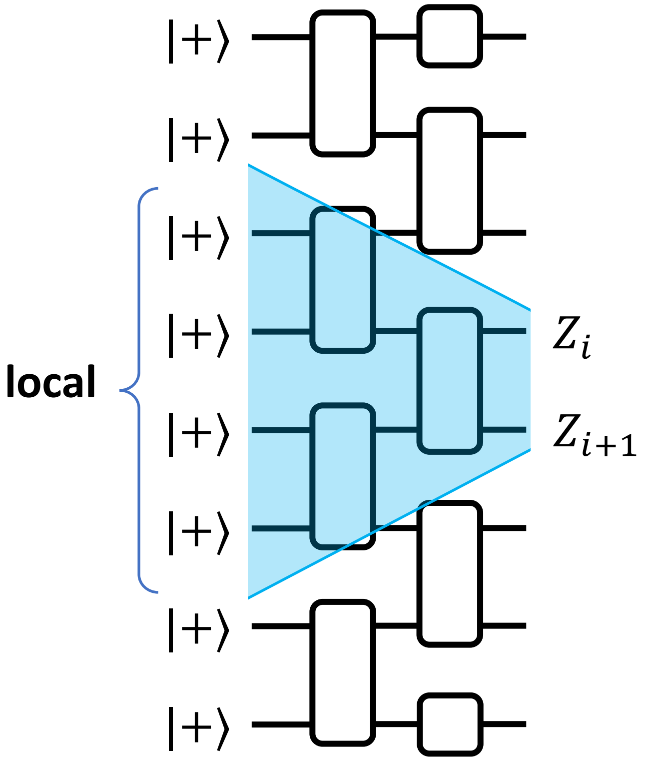
- $p \propto N$: Barren Plateaus(BP) exist. The optimization is hard to perform[McClean, et. al. 2018].



Challenges to QAOA

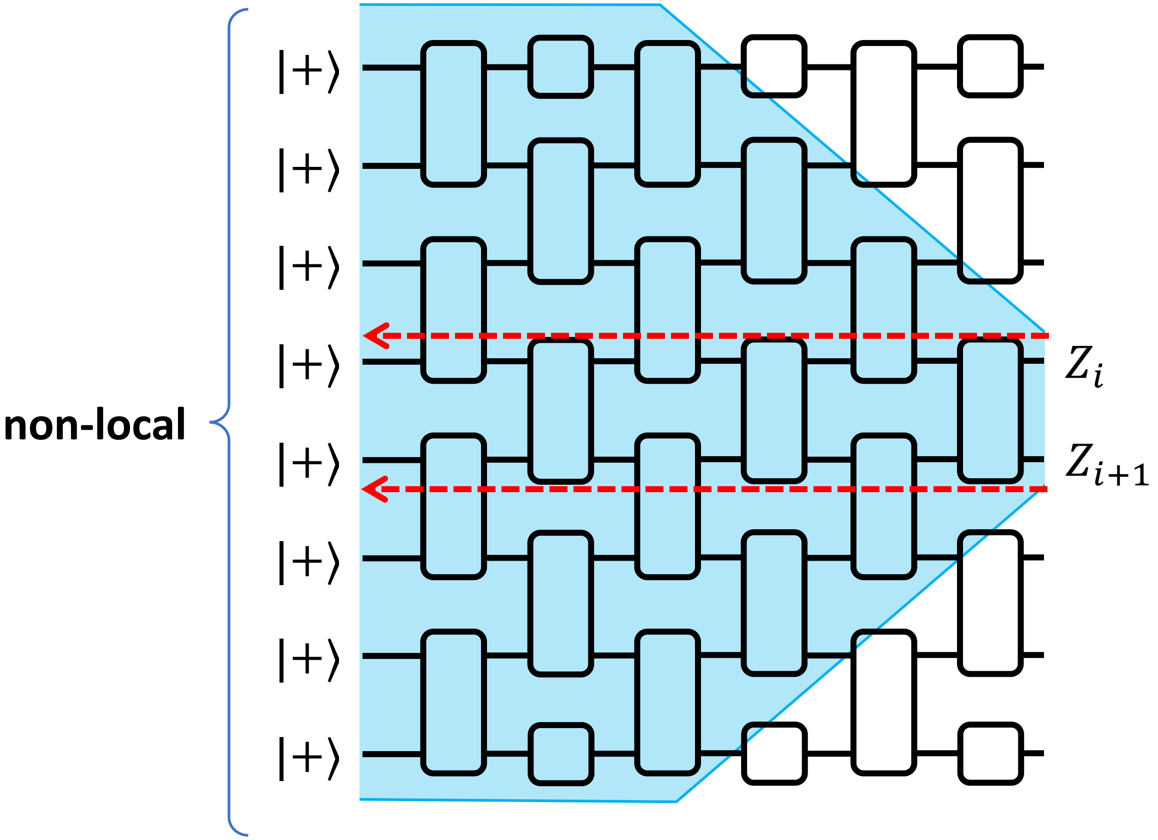
$p = \text{const}$

- For a graph with a constant degree, QAOA is **local**, and **classically simulatable**.

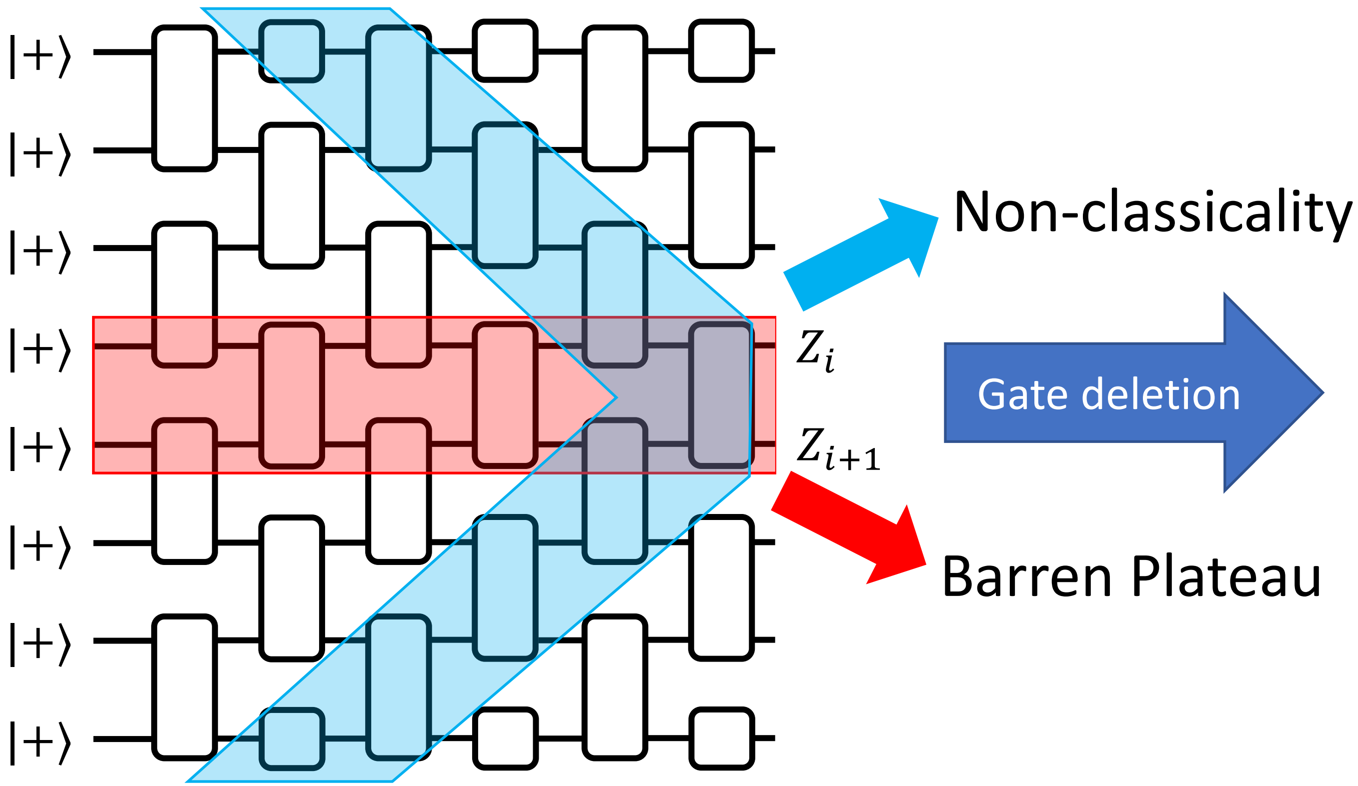


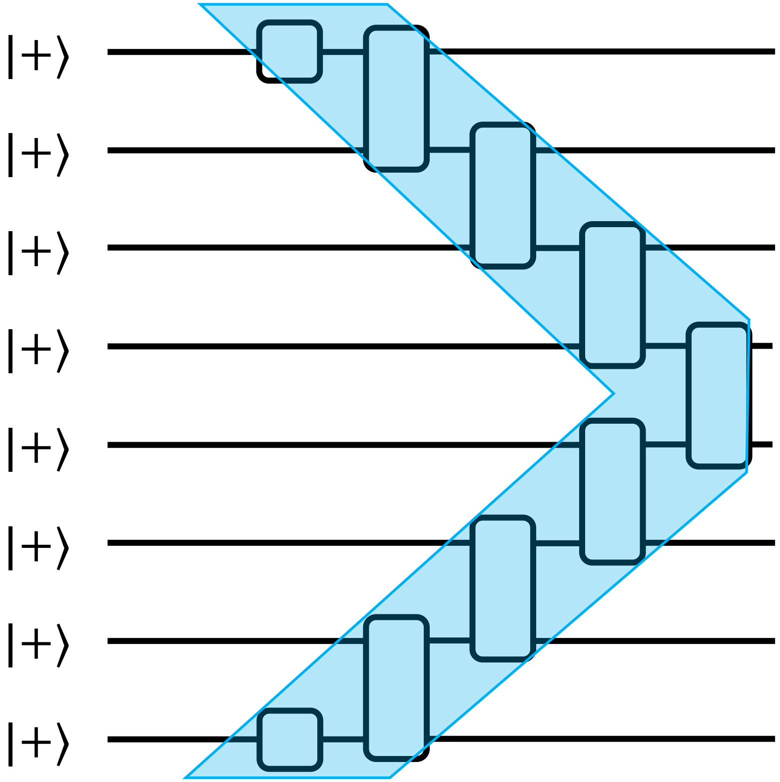
$p \propto N$

- The circuit is **non-local**, and **non-classically simulatable**, but the observable is uncommute with linearly many gates, which leads to **Barren Plateau**.



iHVA-tree ansatz





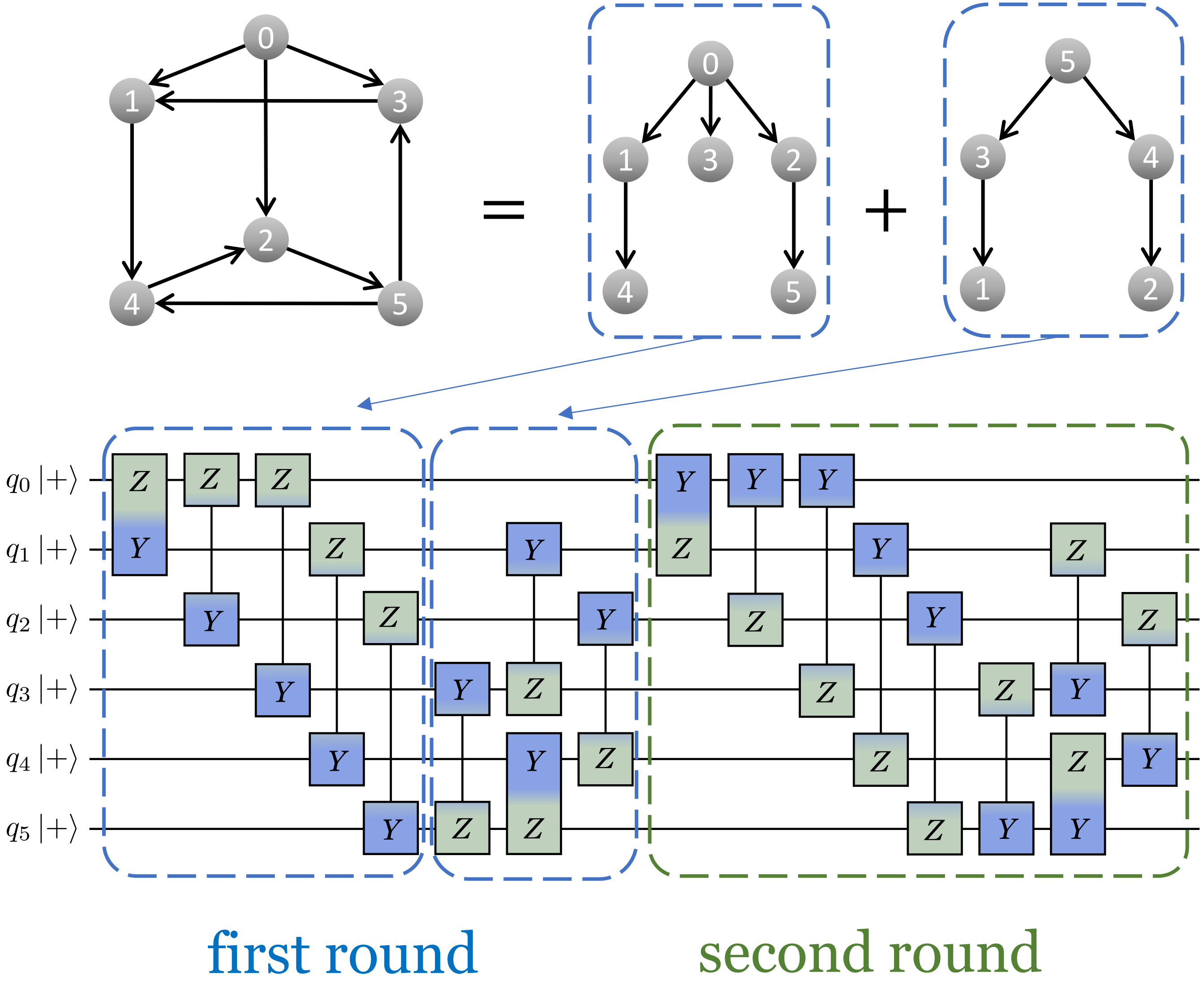
- Non-classicality (necessary for high accuracy)
- Barren Plateau-free (high trainability) *[H. Zhang, et.al. PRL 2024]*

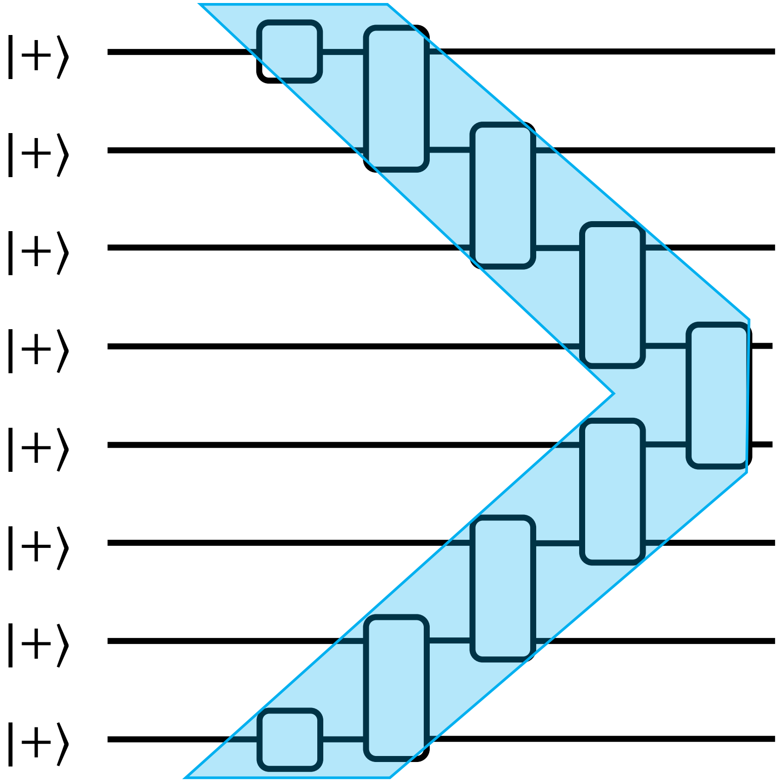
- The light-cone can be constructed by breadth-first search(BFS) for general graphs.

→ BFS-tree

iHVA-tree ansatz

- Construction of the iHVA-tree ansatz.





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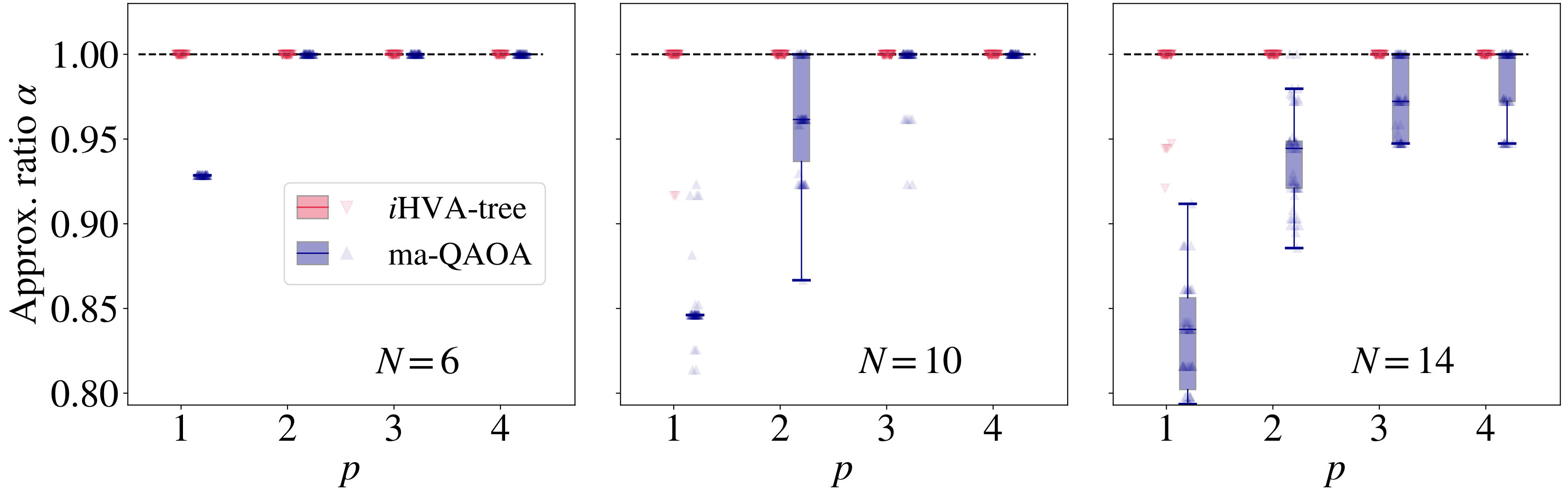
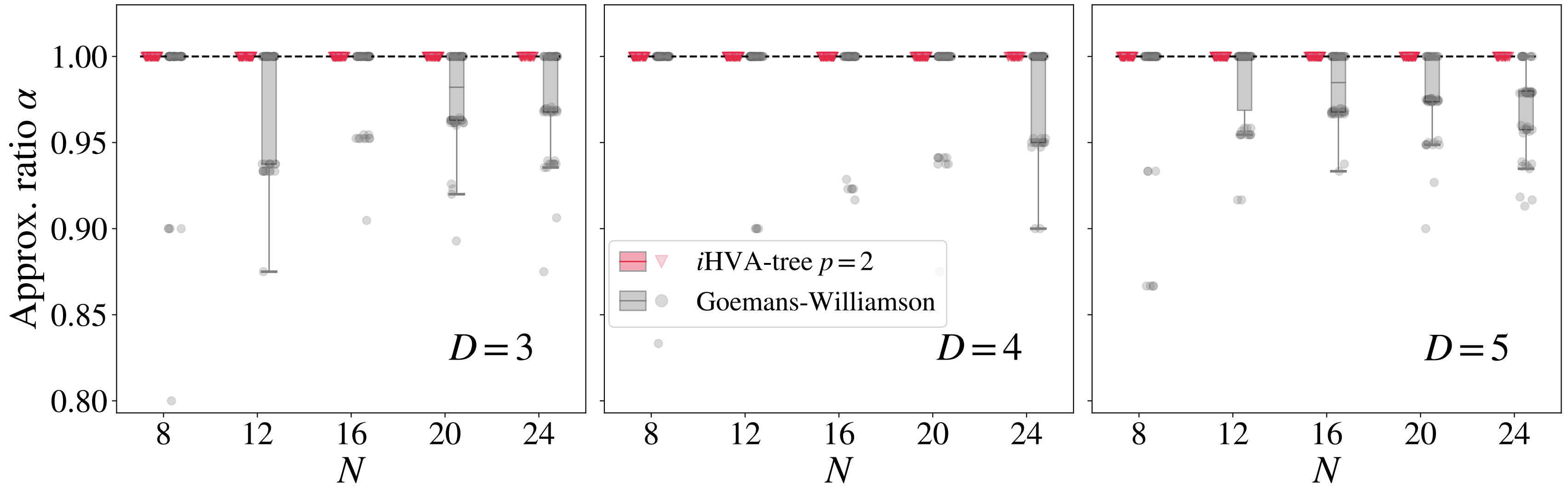
Numerical results on simulator

Compared with QAOA



- iHVA-tree($p \geq 2$) can exactly solve MaxCut of randomly generated 3-regular graphs. While QAOA requires p increasing with N (almost linearly).

Compared with classical algorithm (Goemans-Williamson)



- Up to 24 graph nodes. iHVA-tree ($p = 2$) solves MaxCut of random D-regular graphs exactly. In contrast, the classical algorithm can only derive approximate solutions.

Numerical results on hardware

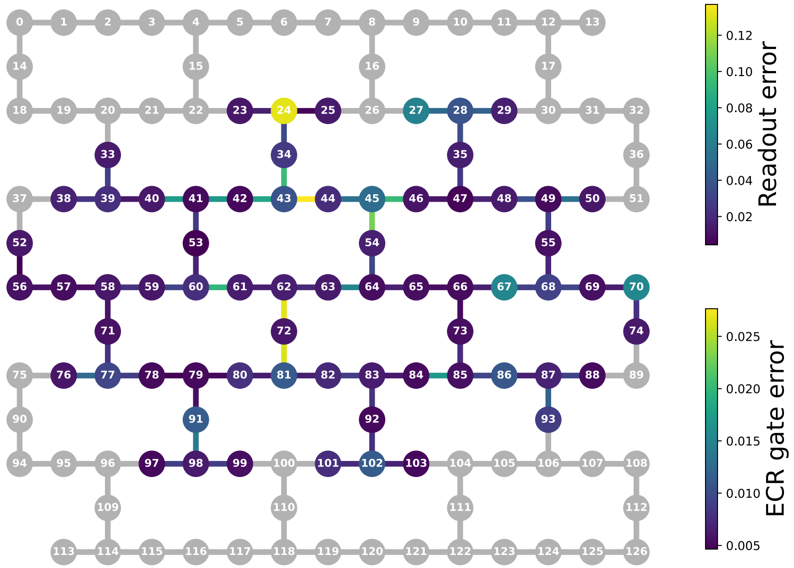
MaxCut experiment (67 Qubits)

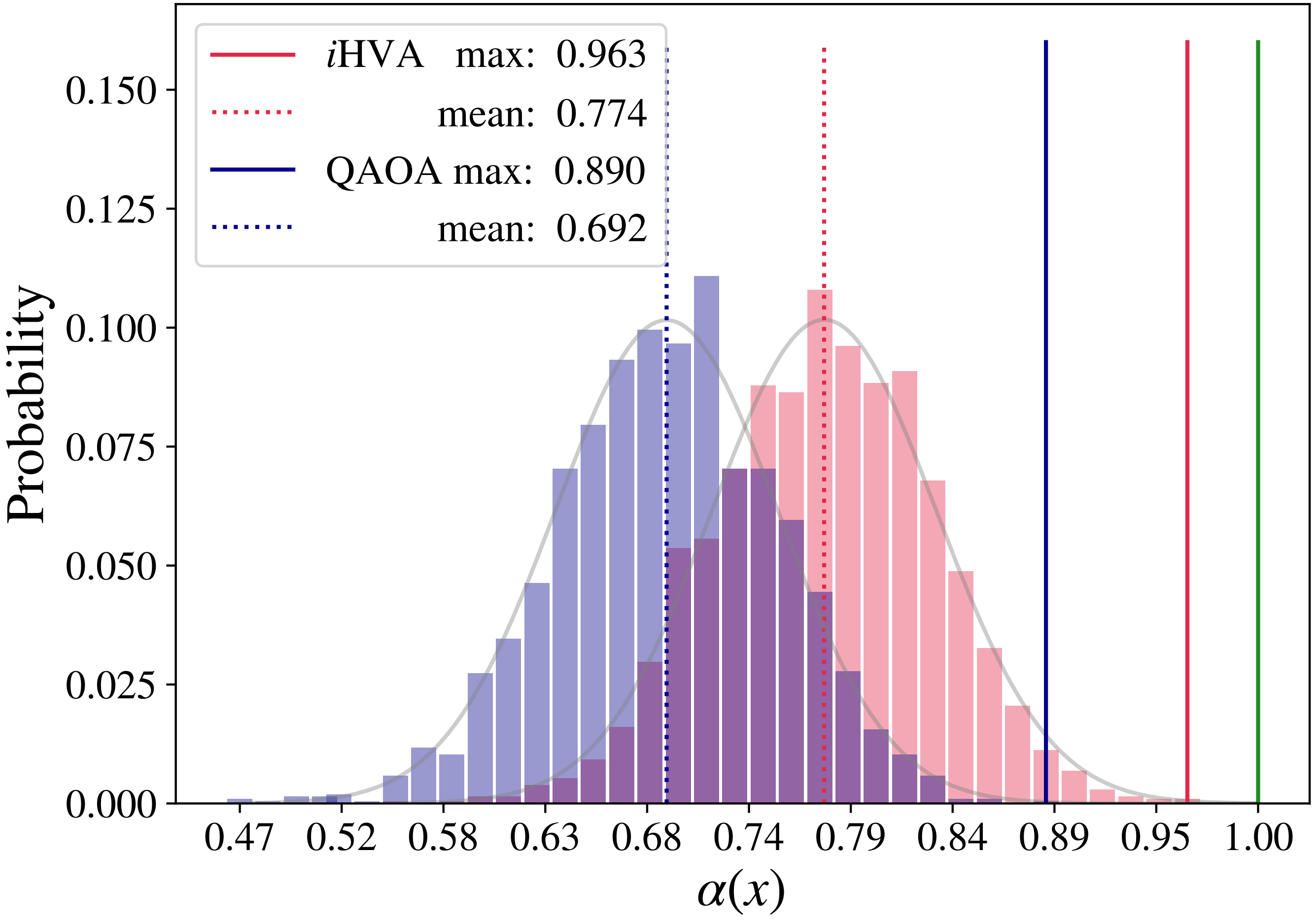
$$H = -\frac{1}{2} \sum_{(i,j)\in\mathcal{E}} (1 - w_{ij} Z_i Z_j) \qquad (w_{ij} = \pm 1)$$

$$|\phi_I(\theta)\rangle = \prod_{(i,j)\in\mathcal{E}} e^{-i\theta w_{ij} Z_i Y_j/2} |+\rangle^{\otimes N}$$

$$|\phi_R(\beta,\gamma)\rangle = \prod_{i\in\mathcal{V}} e^{-i\beta X_i/2} \prod_{(i,j)\in\mathcal{E}} e^{-i\gamma w_{ij} Z_i Z_j/2} |+\rangle^{\otimes N}$$

ibm_brisbane





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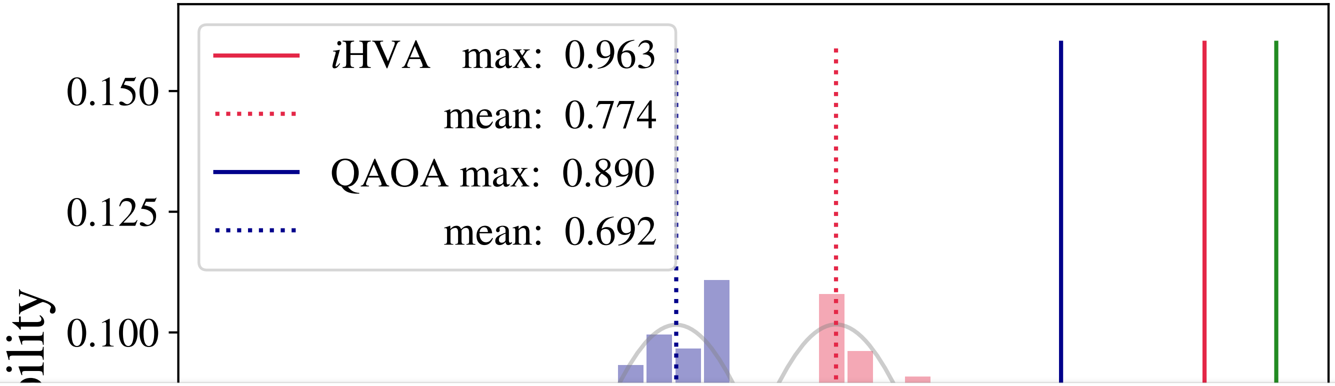
MaxCut experiment (67 Qubits)

$$H = -\frac{1}{2}\sum_{(i,j)\in\mathcal{E}}(1 - w_{ij}Z_iZ_j) \qquad (w_{ij} = \pm 1)$$

$$|\phi_I(\theta)\rangle = \prod_{(i,j)\in\mathcal{E}} e^{-i\theta w_{ij}Z_iY_j/2}\,|+\rangle^{\otimes N}$$

$$|\phi_R(\beta,\gamma)\rangle = \prod_{i\in\mathcal{V}} e^{-i\beta X_i/2} \prod_{(i,j)\in\mathcal{E}} e^{-i\gamma w_{ij}Z_iZ_j/2}\,|+\rangle^{\otimes N}$$

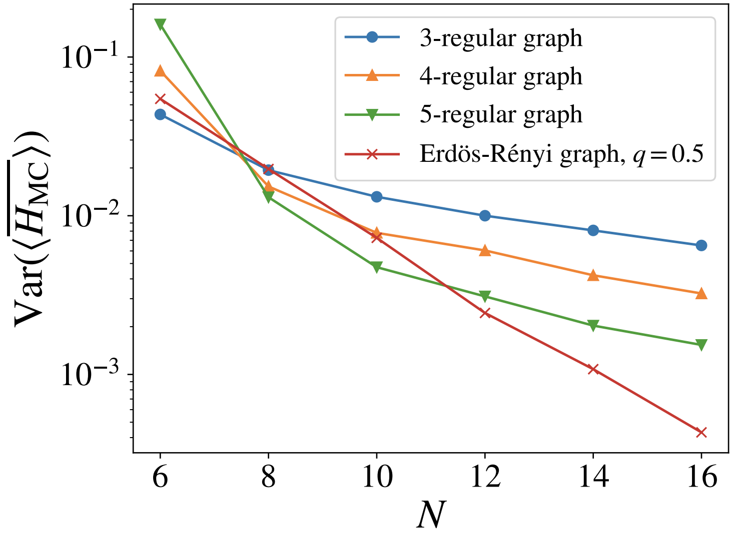


Performance analysis of iHVA

- **Trainability:**

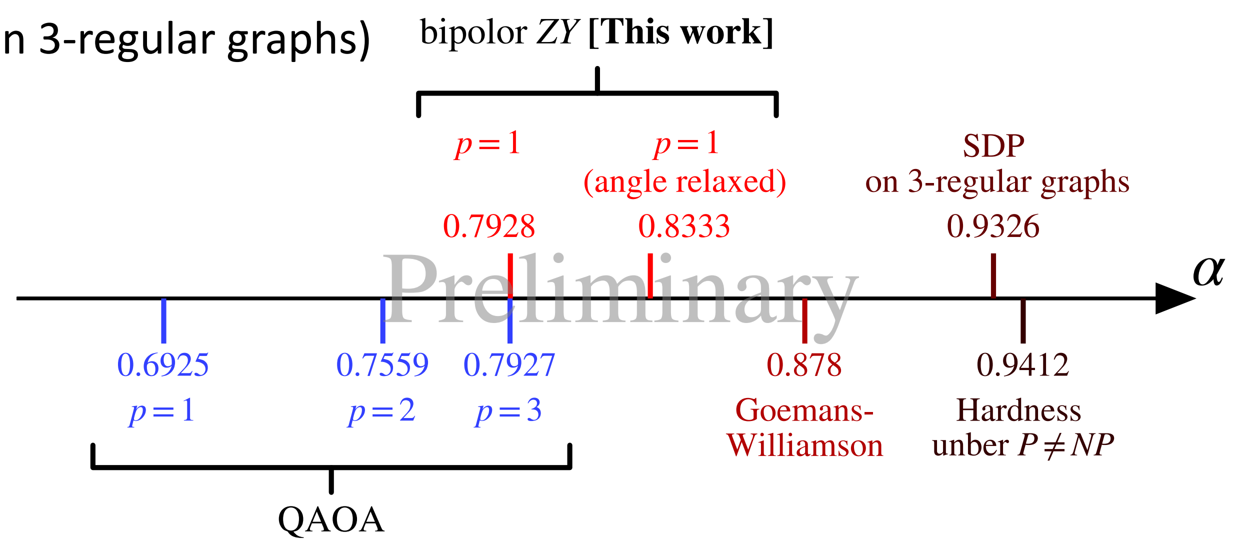
  iHVA of D-regular graph with constant p is
  Barren Plateau-free.

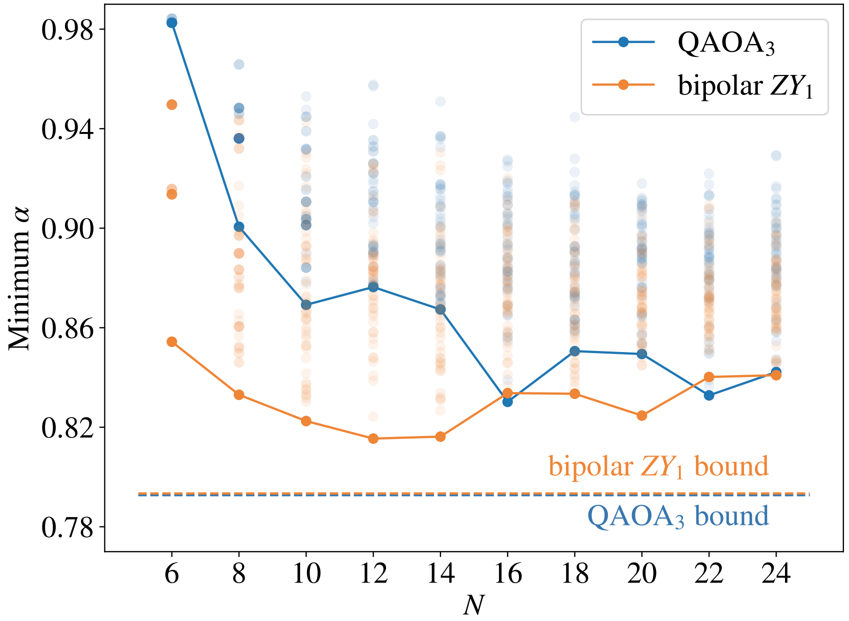
$$\left\|\frac{\partial C(\boldsymbol{\theta})}{\partial \theta_i}\right\| \geq \frac{DN}{E_0^2 2^{D(p+1)-1}} \gg \frac{1}{2^N}$$



- **Solution accuracy:**

(on 3-regular graphs)





1-round iHVA($p = 1$) ⟺ 3-round QAOA ($p = 3$)

Main Content

- QAOA ansatz and its challenges
- imaginary Hamiltonian variational ansatz
- iHVA-tree and its performance on MaxCut
- Conclusion and outlooks

Conclusion and Outlook

Conclusion

- We proposed a systematic method to construct imaginary Hamiltonian Variational Ansatz (iHVA).
- The non-local BFS-tree structure can further improve the solution accuracy.
- Compared with QAOA:
  - iHVA converges faster to the ground state.
  - iHVA-tree has both higher accuracy and higher trainability.

Outlook

- **Numerically**: Solve ground-state problems in larger-scale and more complicated setups
- **Theoretically**: find a theoretical performance bound that could beat the best classical algorithm

} Try to show quantum advantage in real-world applications

ありがとうございます

Thanks for watching!