Parameter optimization strategies in variational quantum algorithms

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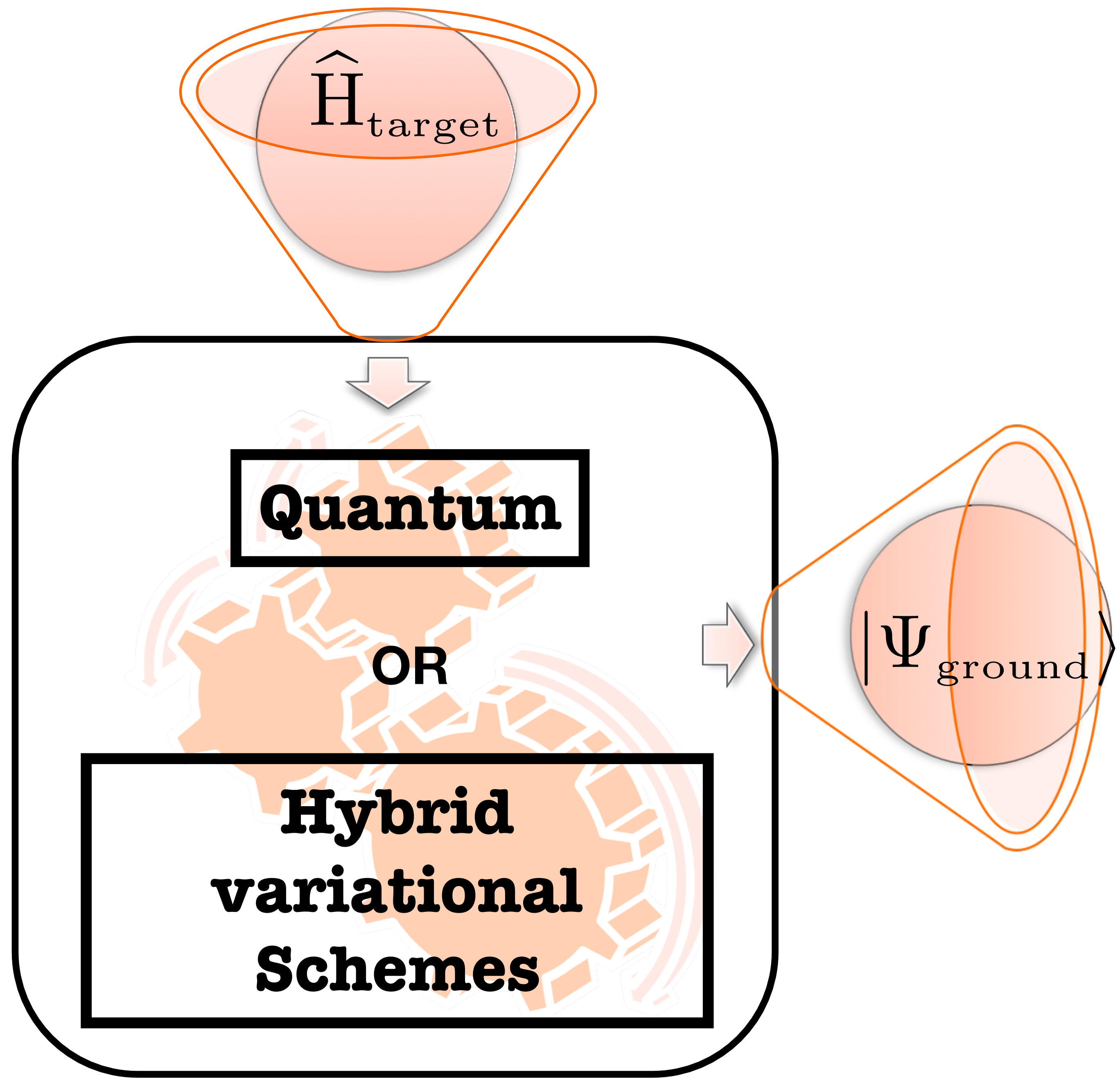
Quantum ground state preparation



Applications

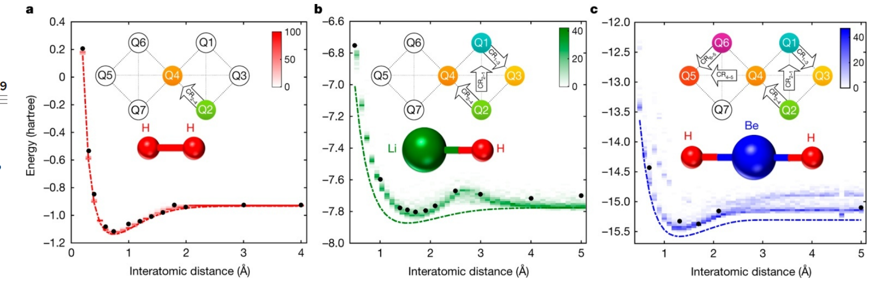
❖**Quantum chemistry**

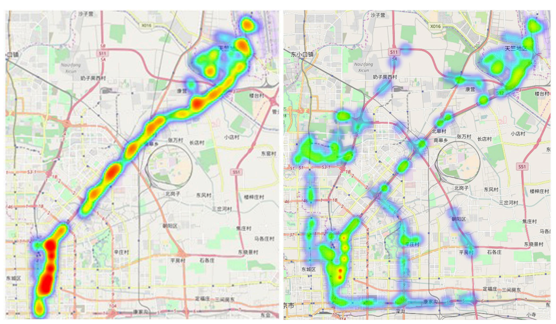
LETTER

doi:10.1038/nature23879

Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets

Abhinav Kandala[1]*, Antonio Mezzacapo[1]*, Kristan Temme[1], Maika Takita[1], Markus Brink[1], Jerry M. Chow[1] & Jay M. Gambetta[1]





Traffic Flow Optimization Using a Quantum Annealer

Florian Neukart[1], Gabriele Compostella[2], Christian Seidel[2], David von Dollen[1], Sheir Yarkoni[3] and Bob Parney[3]*

❖**Computer Science**

❖**Machine learning**

PNAS

Efficiency of quantum vs. classical annealing in nonconvex learning problems

Carlo Baldassi[a,b,1,2] and Riccardo Zecchina[a,c,1,2]

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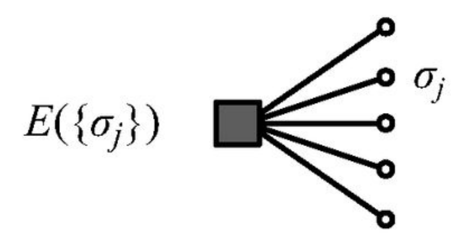
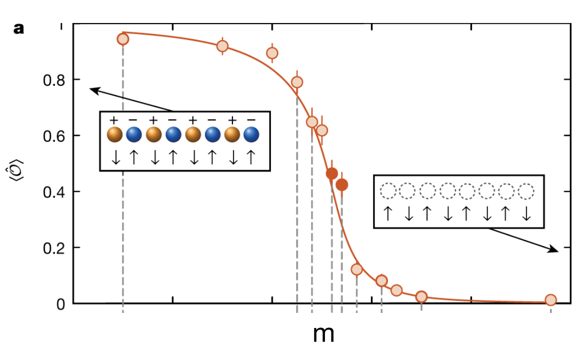
Edited by William Bialek, Princeton University, Princeton, NJ, and approved January 2, 2018 (received for review June 26, 2017)





ARTICLE

https://doi.org/10.1038/s41586-019-1177-4

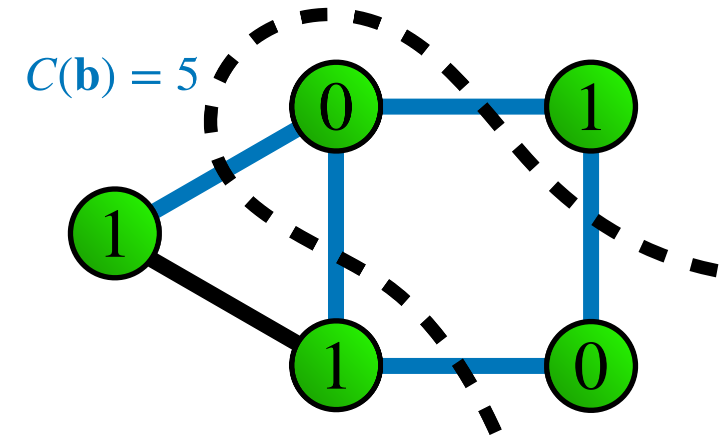
Self-verifying variational quantum simulation of lattice models

C. Kokail[1,2,3], C. Maier[1,2,3], R. van Bijnen[1,2,3], T. Brydges[1,2], M. K. Joshi[1,2], P. Jurcevic[1,2], C. A. Muschik[1,2], P. Silvi[1,2], R. Blatt[1,2], C. F. Roos[1,2] & P. Zoller[1,2]*

❖**Physics**

Quantum Optimization

Combinatorial optimization: Minimization of a single valued function of discrete variables



Examples

MaxCut: $E_{cl}(\mathbf{b}) = -C(\mathbf{b}) = -\sum_{\langle i,j\rangle} (b_i \oplus b_j)$

weighted-MaxCut: $E_{cl}(\mathbf{b}) = -\sum_{\langle i,j\rangle} J_{ij}(b_i \oplus b_j)$

bit: $b = 0,1$

qubit: $|\psi\rangle = a_0|0\rangle + a_1|1\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$

Pauli matrices: $\hat{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{\sigma}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \hat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Optimal configuration?

$E_{cl}(\mathbf{b}) = -\sum_{\langle i,j\rangle} J_{ij}(b_i \oplus b_j)$

$b_j = (1 - \hat{\sigma}^z)/2$

Ground state $|\psi_{\text{ground}}\rangle$?

$$\hat{H}_z = \frac{1}{2}\sum_{\langle i,j\rangle} J_{ij}(\hat{\sigma}^z_i\hat{\sigma}^z_j - 1)$$

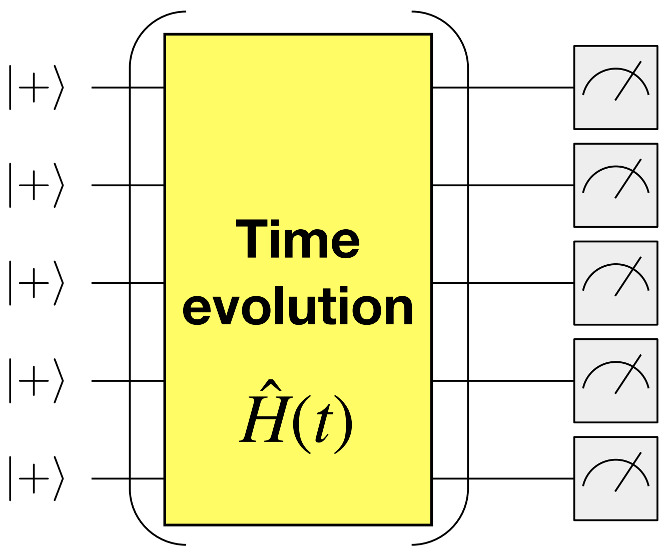
Quantum Optimization

$$\hat{H}_z = \sum_{\langle i,j \rangle} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z$$

Approximate ground state $|\psi_{\text{ground}}\rangle$?

Analog quantum optimization

Review: T. Albash and D. A. Lidar, Rev. Mod. Phys. (2018)

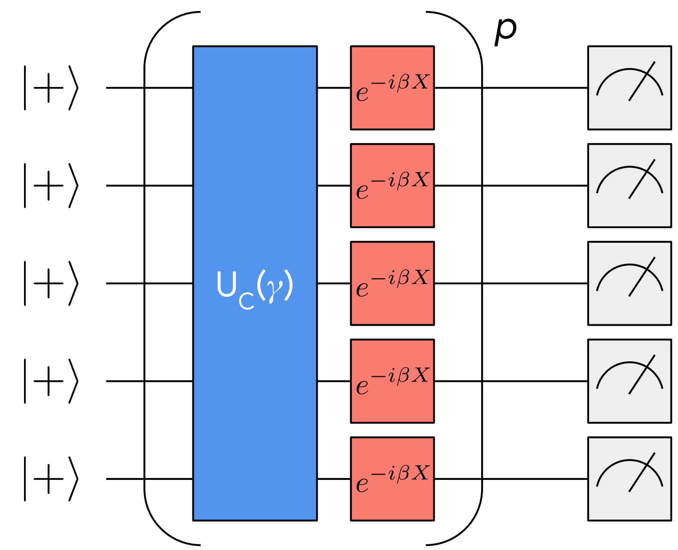


complicated quantum dynamics

$$|\psi_{\text{output}}\rangle = \text{Texp}\left(-\frac{i}{\hbar}\int_0^\tau \hat{H}(t)\mathrm{d}t\right)|\psi_0\rangle$$

Digital quantum optimization

[E. Farhi, *et al*, arXiv:1411.4028 (2014)]



many simple quantum gates

$$|\psi_{\text{output}}\rangle = \ldots \hat{U}_z(\gamma_2)\hat{U}_x(\beta_2)\hat{U}_z(\gamma_1)\hat{U}_x(\beta_1)|\psi_0\rangle$$

Example: quantum search

Grover's problem

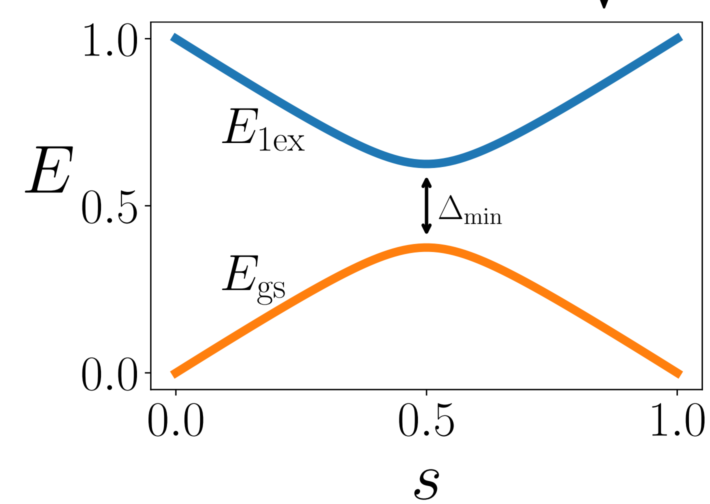
Search an item in an unsorted list of $n = 2^N$ items

Database: binary strings (classical spin configurations) of length N

Marked item: eg. $|\bar{z}\rangle = |\uparrow\downarrow\uparrow\uparrow\downarrow\downarrow\cdots\downarrow\downarrow\uparrow\rangle$

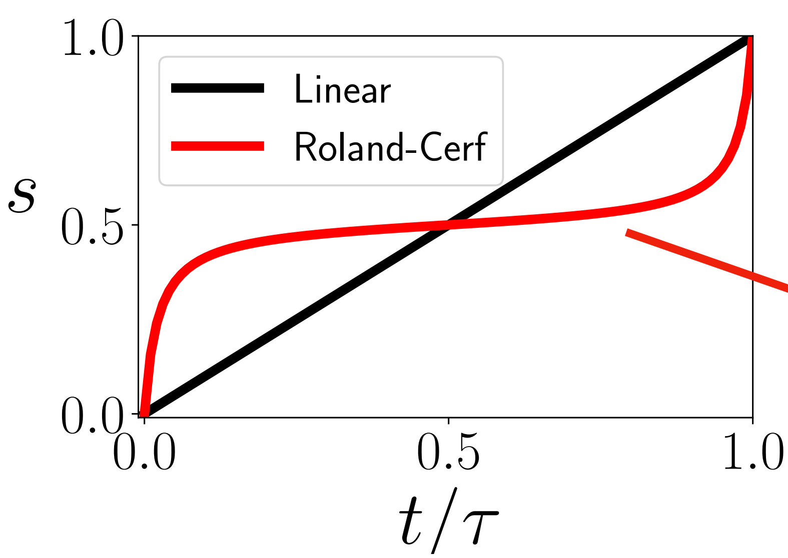
Runtime of classical sequential search: $\tau \propto n$

$$\Delta_{\min} = \Delta(s_c = \frac{1}{2}) = \frac{1}{\sqrt{n}}$$



Quantum Annealing for Grover's problem

$$\widehat{H}(s(t)) = s(t)[\mathbf{1} - |\bar{z}\rangle\langle\bar{z}|] + (1 - s(t))[\mathbf{1} - |+\rangle\langle+|]$$



Linear s(t) (constant speed): $\tau \propto \frac{1}{\Delta^2_{\min}} \propto n$

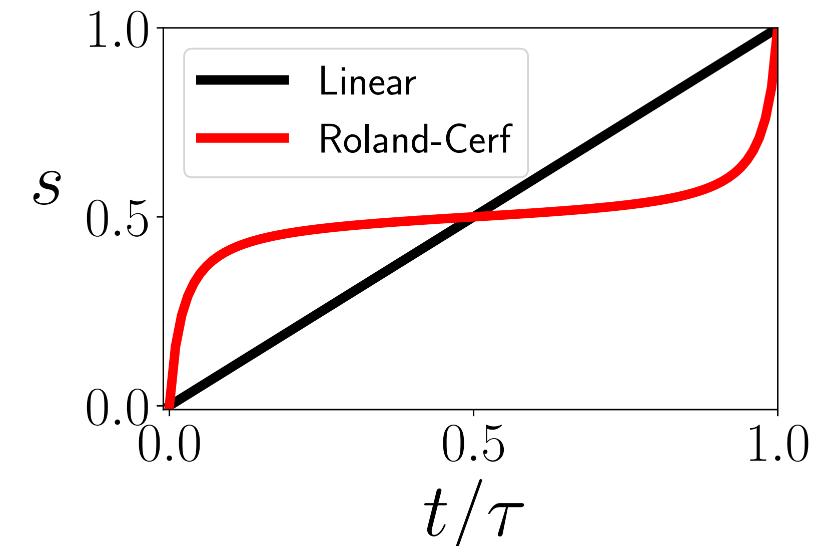
Smart s(t) (slows down near s_c): $\tau \propto \frac{1}{\Delta_{\min}} \propto \sqrt{n}$

[Roland and Cerf, PRA (2002)]

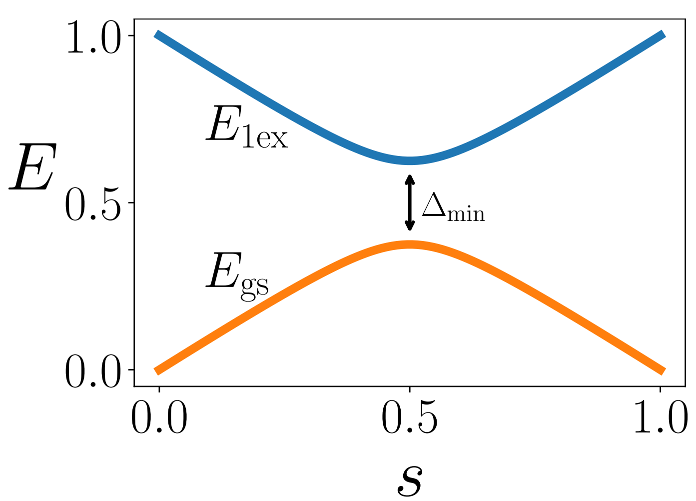
The key role of $s(t)$

Grover's problem

Search an item in an unsorted list of $n = 2^N$ items



Optimal control of the schedule is crucial!



Optimal control of the schedule required spectral information

[Z Jiang, et al PRA (2017)]

How do we do it in general, when spectral information is not available?

[Cubitt et al.,``Undecidability of the spectral gap", Nature (2015)]

Quantum Approximate Optimization

Quantum approximate optimization algorithm

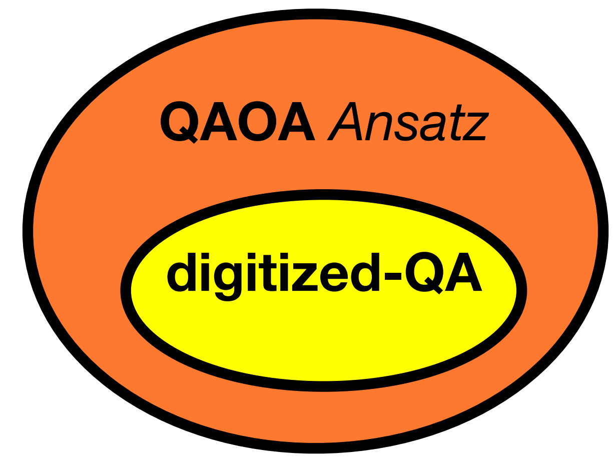
[E. Farhi, *et al*, arXiv:1411.4028 (2014)]
[Blekos, et al Phys. Rep. (2024)]

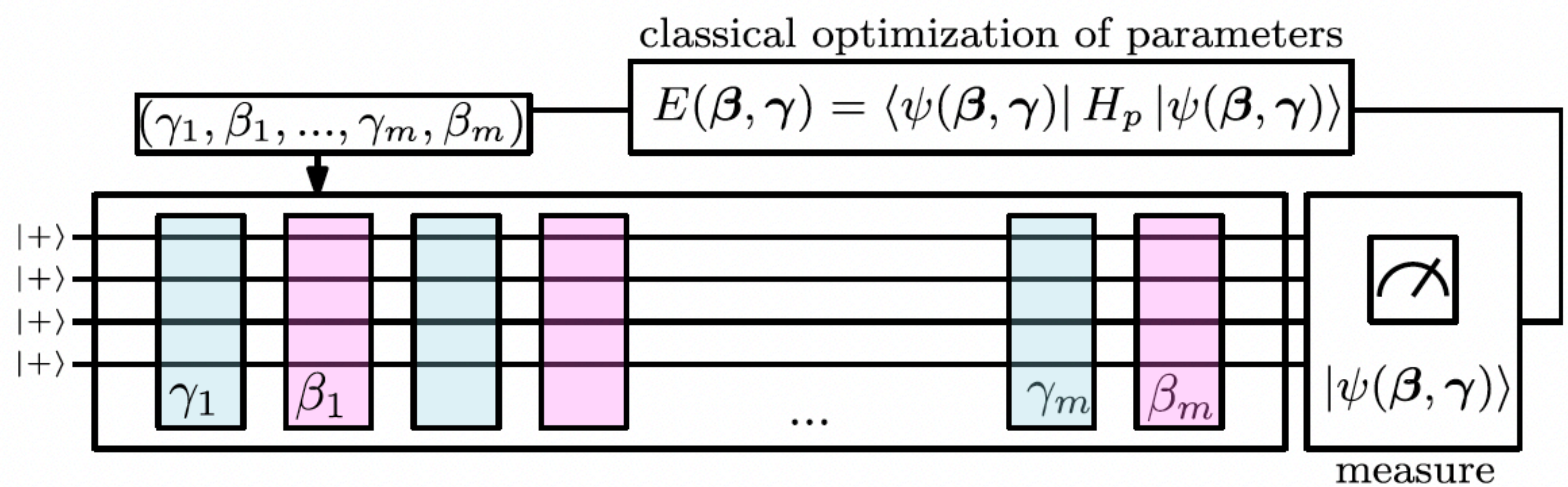
$$U_p(\gamma) = \mathrm{e}^{-i\gamma H_p}$$

$$H_p = H_z = \sum_{i=1}^{N} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z$$

$$U_x(\beta) = \mathrm{e}^{-i\beta H_x}$$

$$H_x = -\sum_{i=1}^{N} \hat{\sigma}_i^x$$





Barren plateaus in quantum neural networks

ARTICLE

DOI: 10.1038/s41467-018-07090-4 OPEN

Barren plateaus in quantum neural network training landscapes

Jarrod R. McClean[1], Sergio Boixo[1], Vadim N. Smelyanskiy[1], Ryan Babbush[1] & Hartmut Neven[1]

ARTICLE

https://doi.org/10.1038/s41467-021-21728-w OPEN

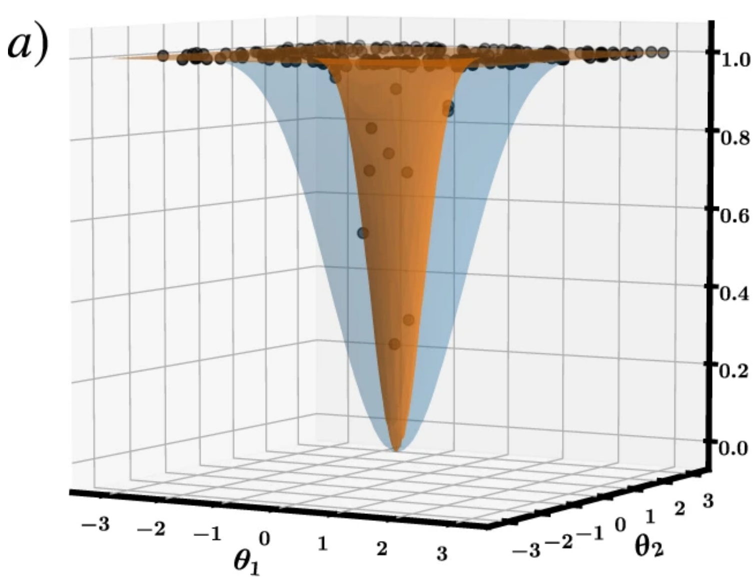
Check for updates

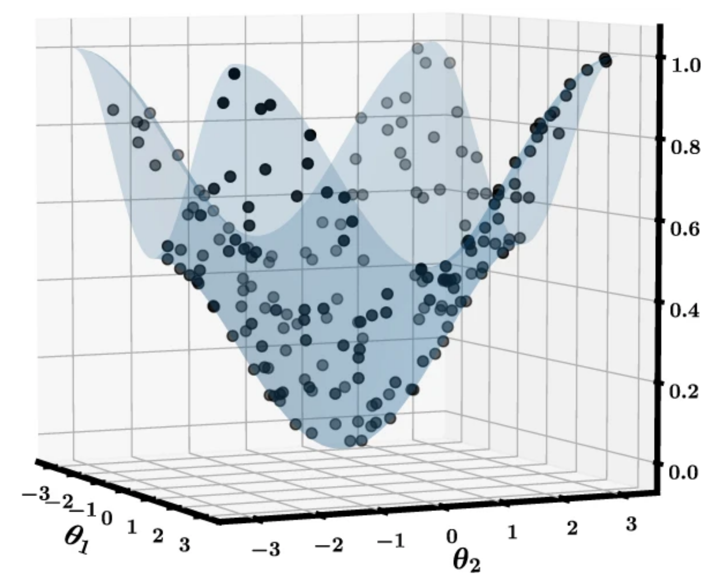
Cost function dependent barren plateaus in shallow parametrized quantum circuits

M. Cerezo[1,2✉], Akira Sone[1,2], Tyler Volkoff[1], Lukasz Cincio[1] & Patrick J. Coles[1✉]

Gradient of the cost function $\nabla E = \left(\frac{\partial E}{\partial \gamma_1}, \frac{\partial E}{\partial \gamma_2} \ldots \frac{\partial E}{\partial \beta_1} \frac{\partial E}{\partial \beta_2} \ldots \right)$

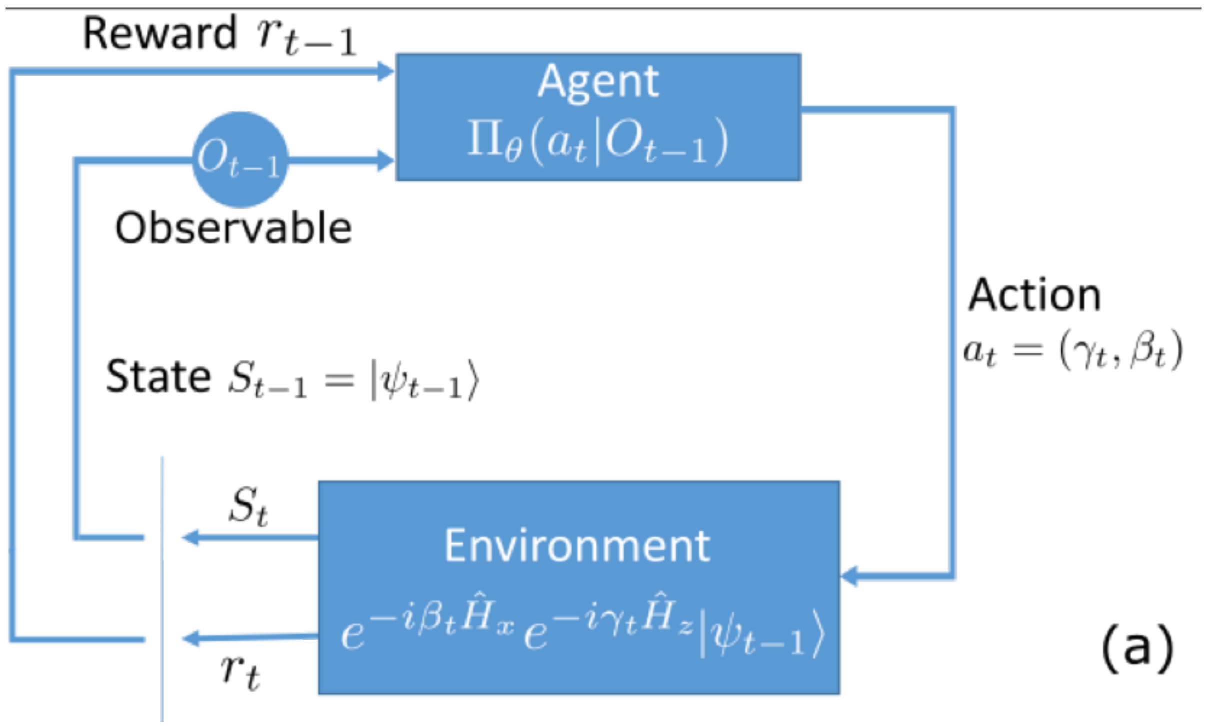
$$\mathrm{Var}\left[\frac{\partial E}{\partial \theta}\right] \to 0 \qquad\qquad \mathrm{Var}\left[\frac{\partial E}{\partial \theta}\right] \neq 0$$





QAOA as Markov decision process

[Wauters, et al., Phys. Rev. Res. (2020)]



Proximal Policy Optimization (PPO)

RL library: https://spinningup.openai.com

Quantum env: https://github.com/mwauters92/QuantumRL

episode → $|\psi_0\rangle$ through $|\psi_P\rangle$
state **S** → instantaneous $|\psi_t\rangle$
observable **O** → $\langle\psi_t|O|\psi_t\rangle$
action **A** → (γ_m, β_m)
reward **R** → $r = -\delta_{t,P}\langle\psi_t|\,\widehat{\mathrm{H}}_{\mathrm{target}}\,|\psi_t\rangle$

Two Observables

$O^{(z)} = \langle\psi_t|\,\widehat{H}_z\,|\psi_t\rangle$

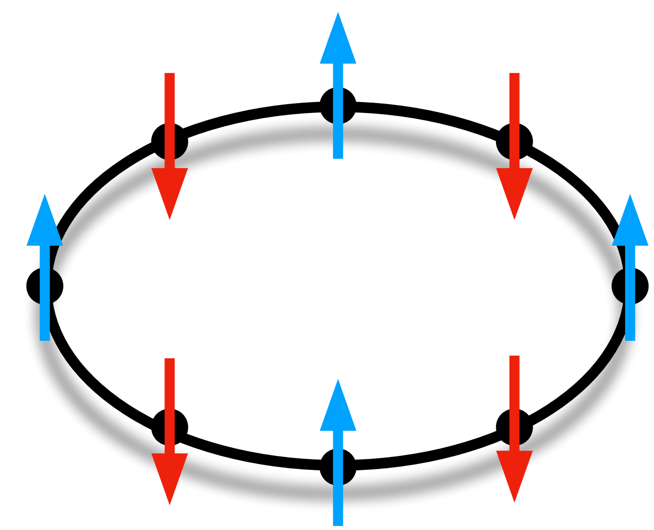
$O^{(x)} = \langle\psi_t|\,\widehat{H}_x\,|\psi_t\rangle$

Require multiple **quantum measurements**!

Quantum Ising Chain/Ring of disagrees

$$\widehat{\mathrm{H}}_{\text{target}} = \widehat{H}_z + \cancel{h\widehat{H}_x}$$

$$\widehat{H}_x = -\sum_{i=1}^{N} \hat{\sigma}_i^x \qquad \widehat{H}_z = \sum_{i=1}^{N} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z$$



$$\hat{U}_m = \mathrm{e}^{-i\beta_m \widehat{H}_x} \mathrm{e}^{-i\gamma_m \widehat{H}_z}$$

$$|\psi_{\mathrm{P}}(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle = \hat{U}_{\mathrm{P}} \cdots \hat{U}_2 \hat{U}_1 |\psi_0\rangle$$

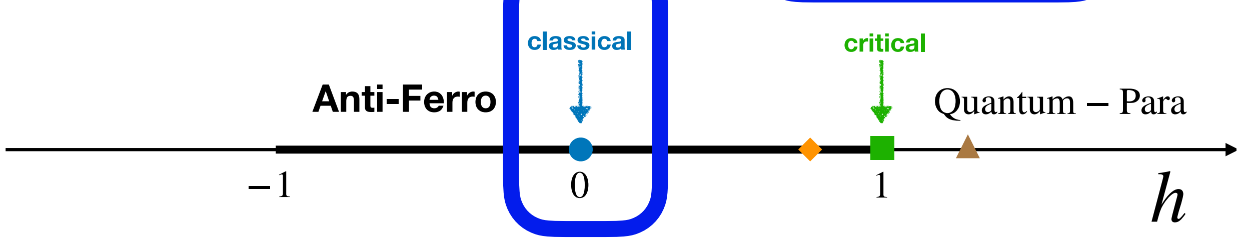
$$E_{\mathrm{P}}(\boldsymbol{\gamma},\boldsymbol{\beta}) = \langle \psi_{\mathrm{P}}(\boldsymbol{\gamma},\boldsymbol{\beta}) | \widehat{H}_{\text{target}} | \psi_{\mathrm{P}}(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle$$

$$E_{\min} = -N \qquad E_{\max} = N$$

residual energy
(relative **error**)

$$\epsilon_{\mathrm{P}}^{\text{res}}(\boldsymbol{\gamma},\boldsymbol{\beta}) = \frac{E_{\mathrm{P}}(\boldsymbol{\gamma},\boldsymbol{\beta}) - E_{\min}}{E_{\max} - E_{\min}} \in [0,1]$$

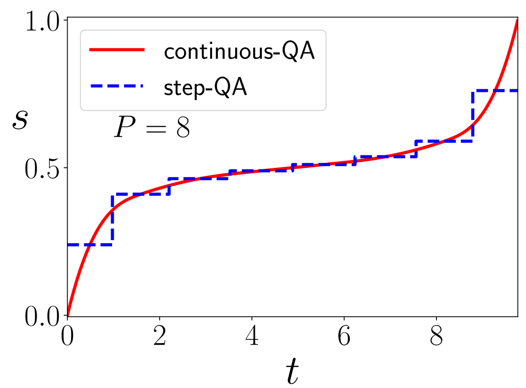
$$h = 0$$



Translationally invariant Ising Chain

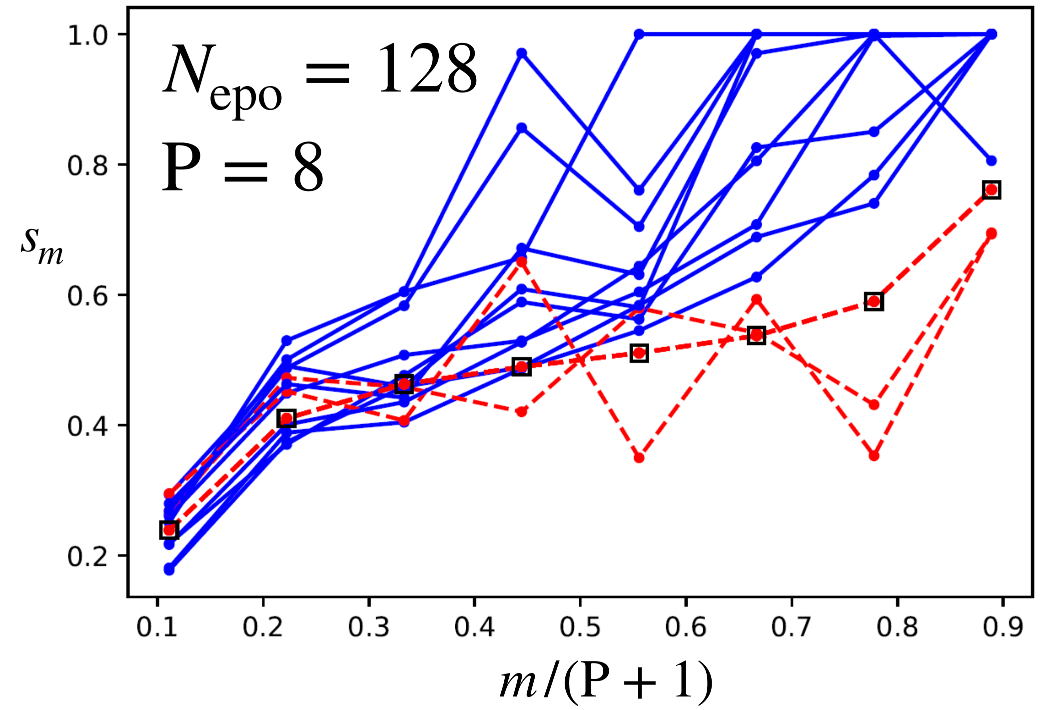
Analyze action choice

$$s_m = \frac{\gamma_m}{\beta_m + \gamma_m}$$



Allows comparison with digital-QA schedule

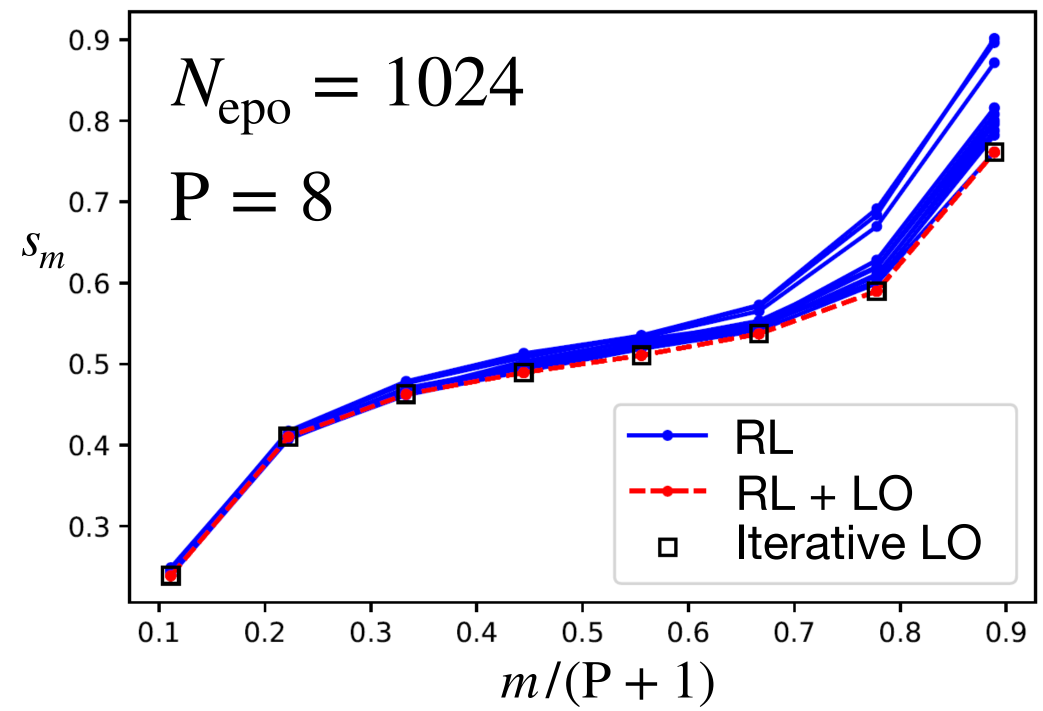
$$\widehat{H}(s_m) = s_m \widehat{\mathrm{H}}_{\text{target}} + (1 - s_m)\widehat{\mathrm{H}}_{\text{driving}}$$



I. Random action choices

II. Large trajectory dispersion. RL+LO fall on the same smooth minimum (iterative LO)

III. RL converges to QAOA iterative solution

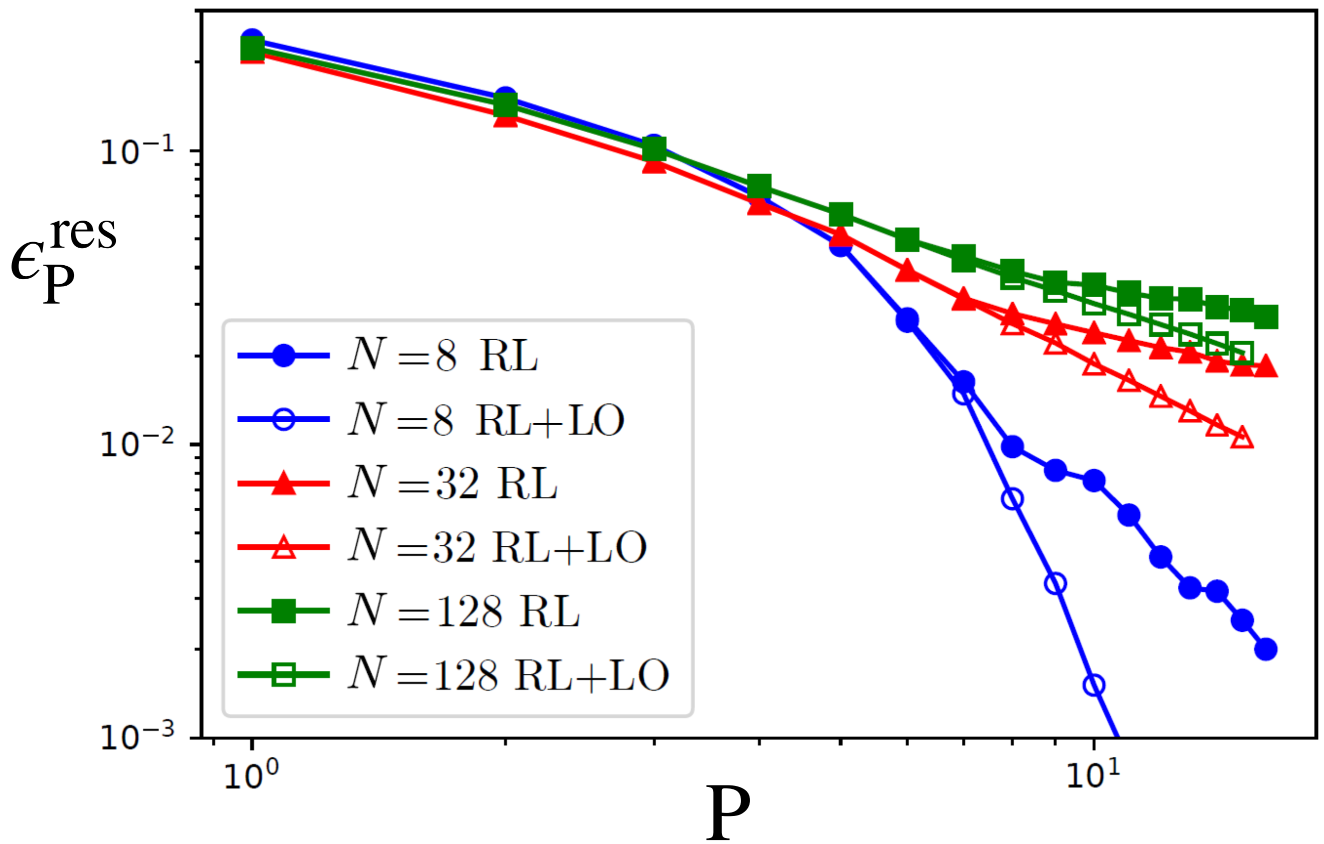


Random Ising Chain

$$\widehat{H}_z = \sum_{i=1}^{N} J_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z$$

J_i Uniformly disturbed in $[0,1]$

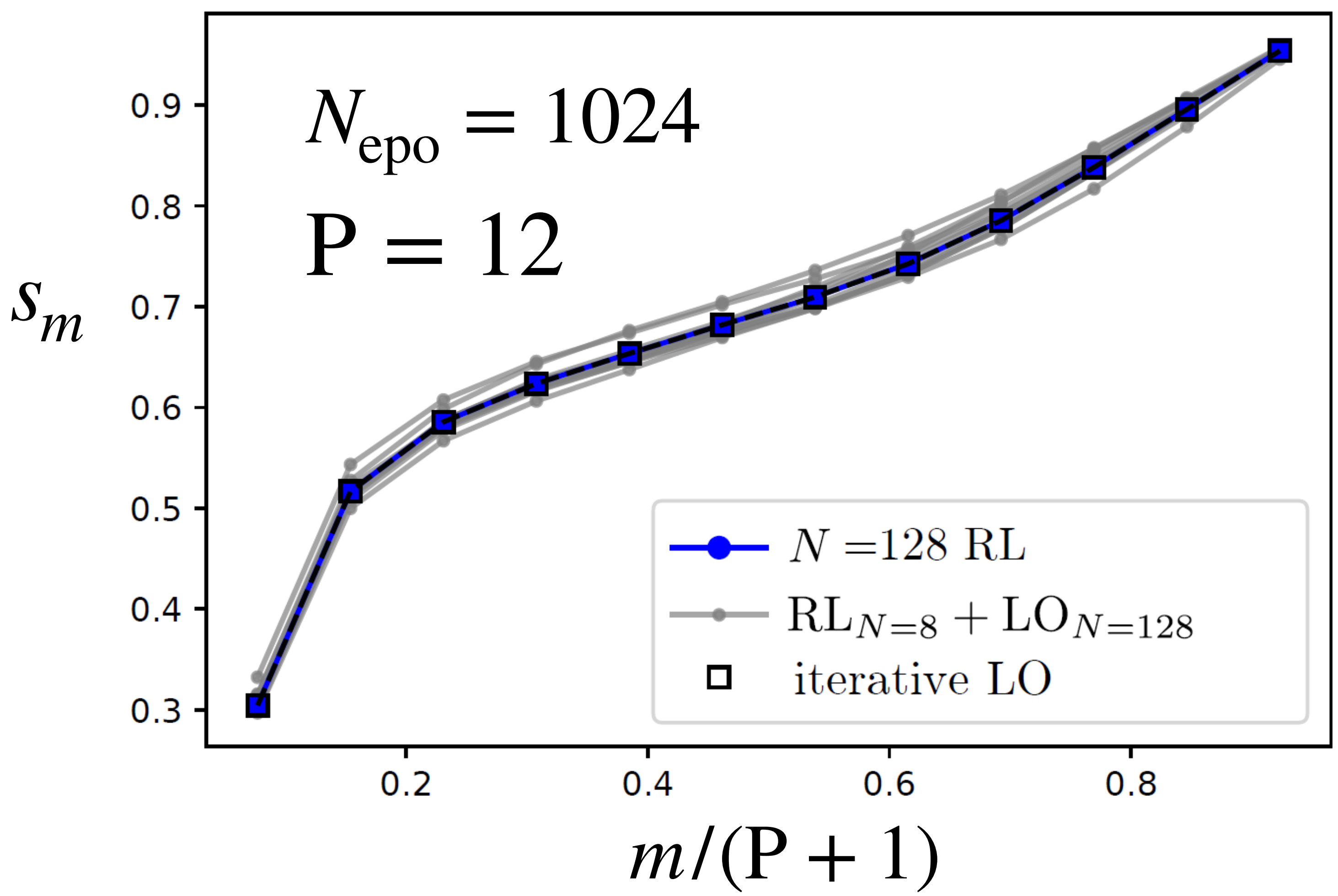
Makes the problem harder



Same phenomenology of uniform TFIM: Local optimization leads to lower energy for P > 6

Open issues:
- No analytical result
- Is solution optimal?
- Better than QA?

Random Ising Chain (transferability)



Policy transferability:

I. Train a small system ($N = 8$) on single disorder instance

II. Get approximate solution $(\boldsymbol{\gamma}^\star, \boldsymbol{\beta}^\star)_{N=8}$

III. Use $(\boldsymbol{\gamma}^\star, \boldsymbol{\beta}^\star)_{N=8}$ to initialize a local optimization on larger system ($N = 128$)

III. RL converges to QAOA iterative solution

Reduces used quantum resources

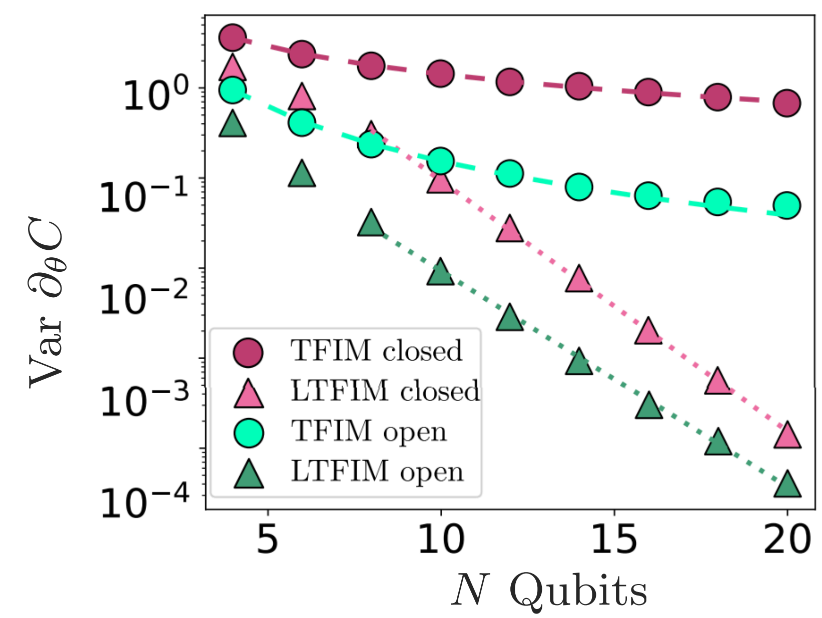
Construction of digitized-QA schedules

Barren plateaus problem

[McClean, et al, PRA (2018)]
[Larocca, et al, Quatum (2022)]

$$\hat{H}_T = \sum_{j=1}^{N} \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z - g_x \sum_{j=1}^{N} \hat{\sigma}_j^x - g_z \sum_{j=1}^{N} \hat{\sigma}_j^z$$

- Gradients vanish exponentially (flat landscape)

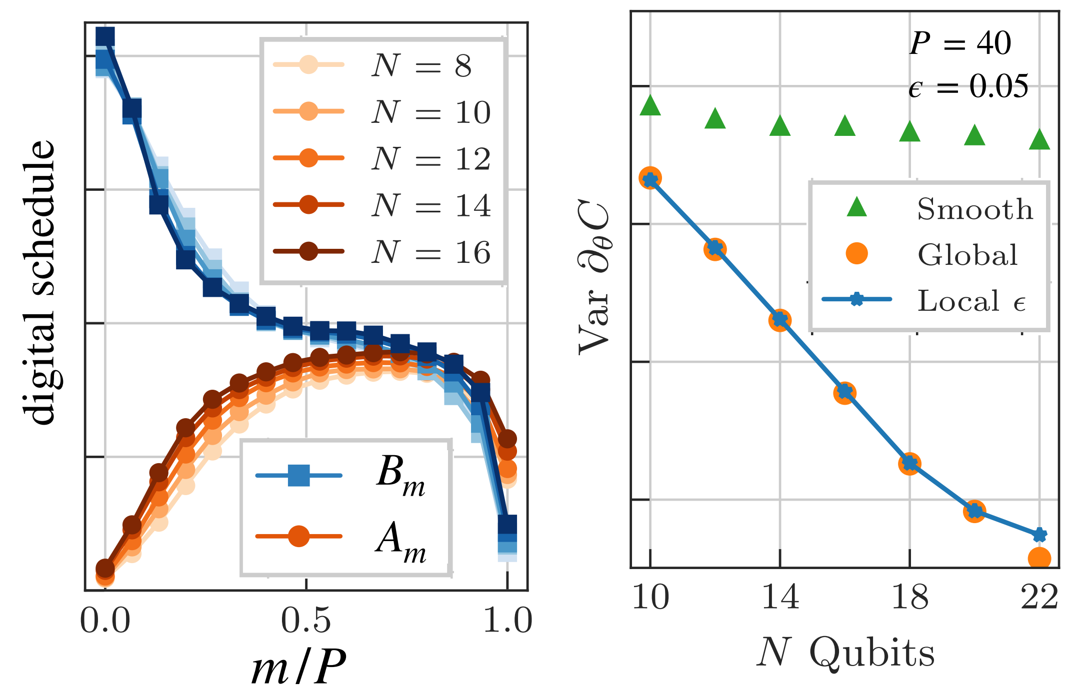


Smooth schedules

[Mele, et al, PRA (2022)]
[Torta, et. Al PRB (2022)]

- Gradients in a neighbourhood of radius ϵ
- Transferred smooth schedule avoids barren plateaus

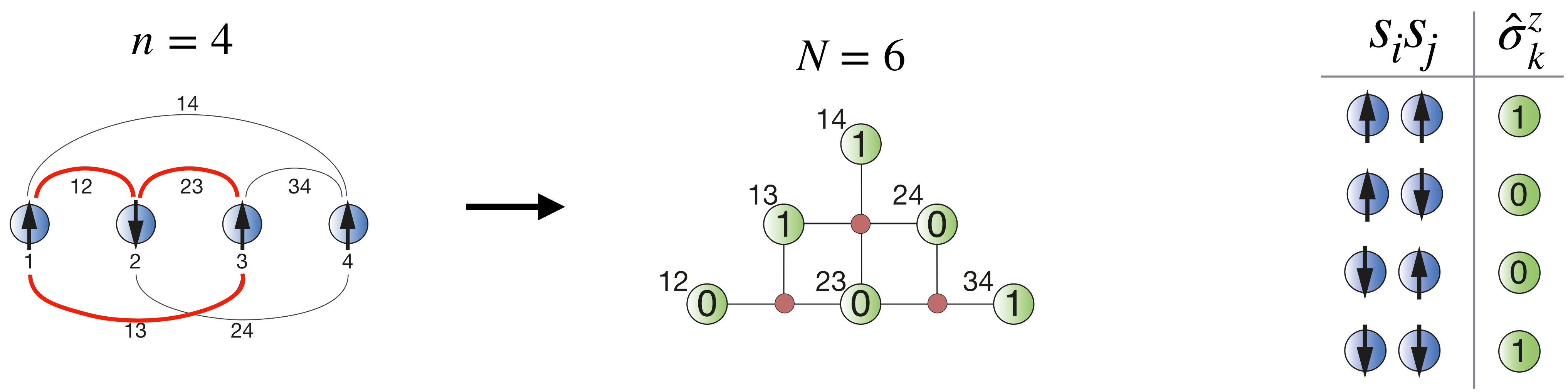
$g_z = g_x = 1$



Hardware challenge: Connectivity

Parity Architecture

[Lechner, Hauke, and Zoller, Sci. Adv. 1, (2015)]



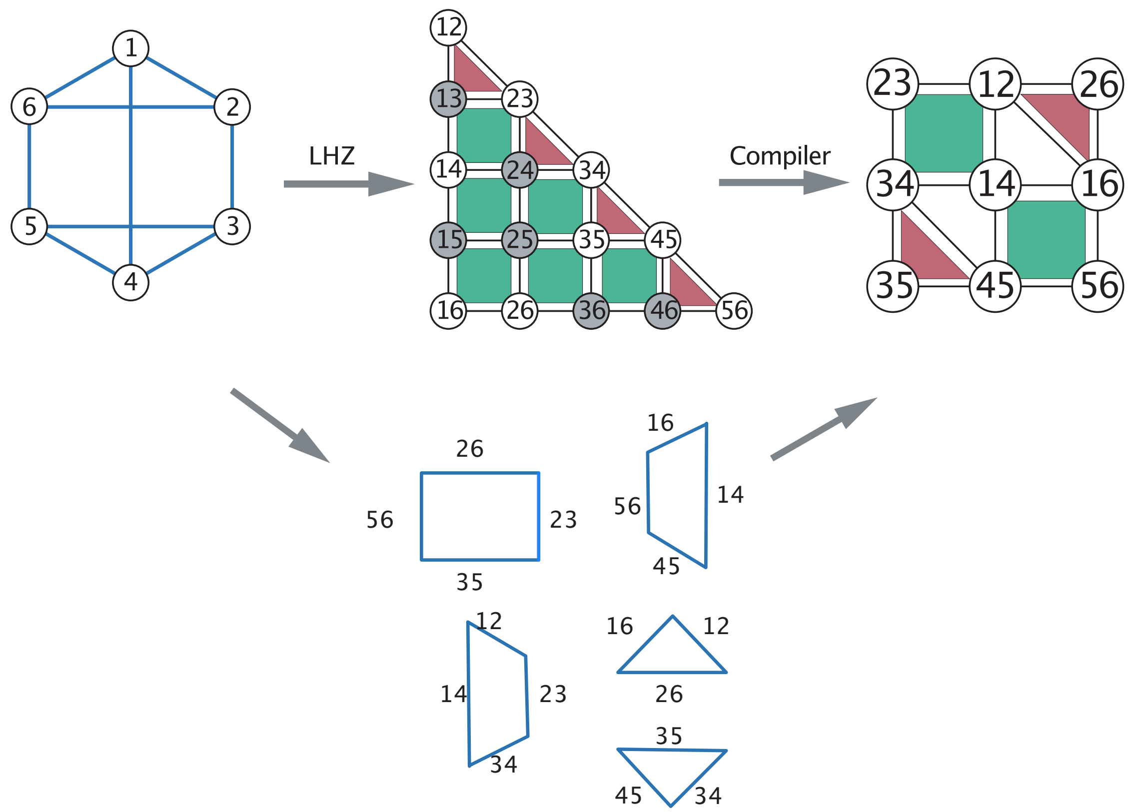
$$H_P = \sum_{i=1}^{n} \sum_{j=1}^{i-1} J_{ij} s_i s_j \longrightarrow H_{\text{LHZ}} = \underbrace{\sum_{i=1}^{N} J_i \hat{\sigma}^z_i}_{\hat{H}_z} + C \underbrace{\sum_{l=1}^{L} (1 - \hat{\sigma}^z_{l_1} \hat{\sigma}^z_{l_2} \hat{\sigma}^z_{l_3} [\hat{\sigma}^z_{l_4}])}_{\hat{H}_C}$$

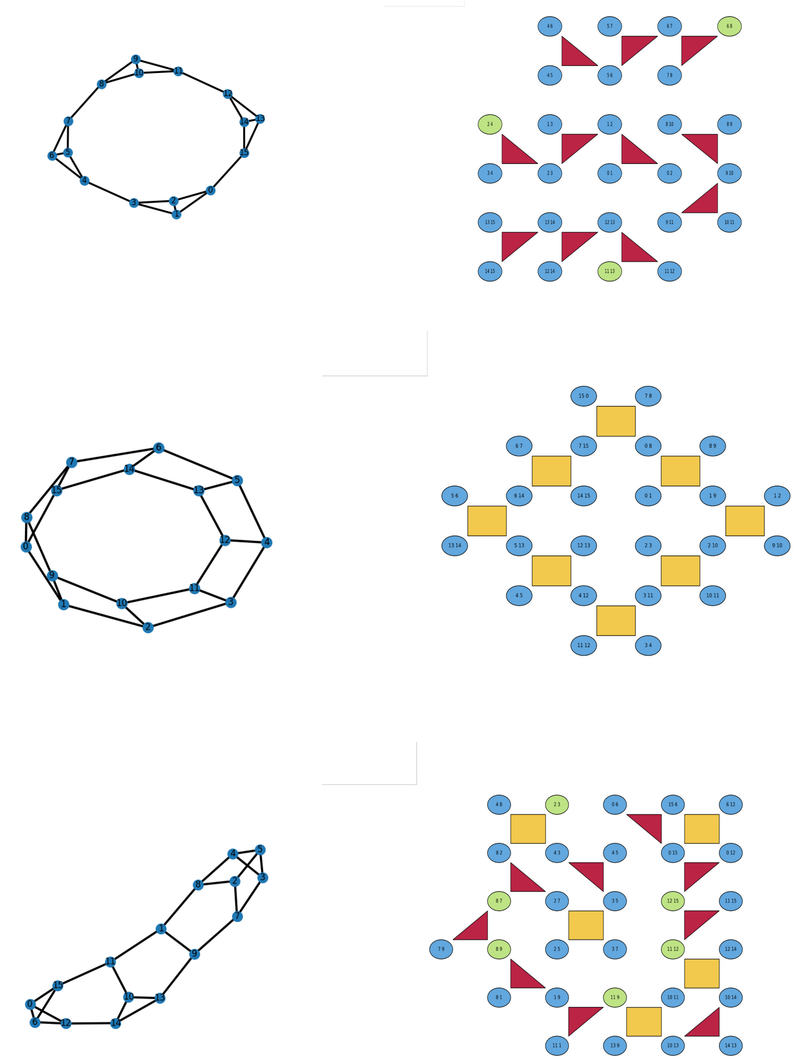
- ❖ The LHZ architecture maps an all-to-all connected spin model to a spin model with only **quasi-local** interactions.
- ❖ The physical qubits encode the **parity** of the logical qubits.
- ❖ **No long-range interactions** but only local 3- or 4-body couplings are necessary.
- ❖ The parity architecture requires nearest-neighbour interactions on a **square lattice**, regardless of the qubit platform.

Parity compilation

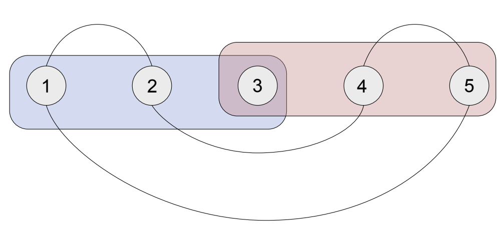
[Ender, et al, Quantum (2023)]

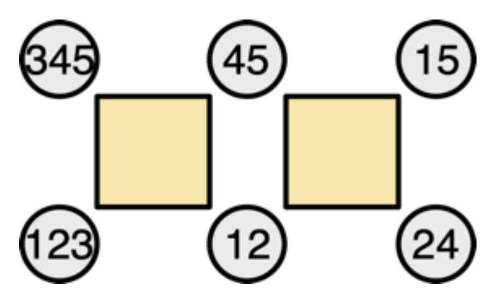
Sparse graphs





Hypergraphs





Parity based QAOA

[Lechner, IEEE Trans. Quantum Eng. (2020)]
[Fellner, et al., PRL (2022)]
[Ender, et al. arXiv (2021)]

$$\tilde{U}_c(\gamma) = e^{-i\Omega \tilde{H}_c}$$

$$\tilde{U}_p(\gamma) = e^{-i\gamma \tilde{H}_P}$$

$$\tilde{U}_x(\beta) = \prod_j e^{-i\beta \tilde{\sigma}_j^x}$$

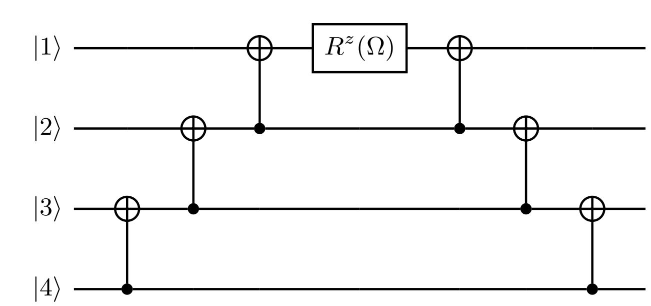
Parity QAOA ansatz:

$$|\psi(\boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{\Omega})\rangle = \tilde{U}_x(\beta_p)\tilde{U}_P(\gamma_p)\tilde{U}_c(\Omega_p) \cdots \tilde{U}_x(\beta_1)\hat{U}_P(\gamma_1)\tilde{U}_c(\Omega_1)|\psi_0\rangle$$

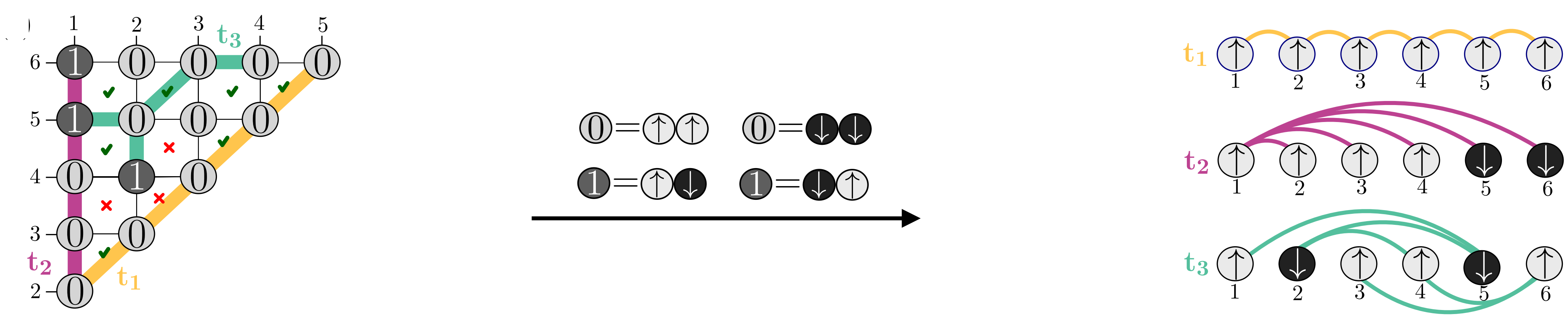
- Fully **parallelizable**
- Generalisation to **k-body terms**
- Uses fewer **CNOT gates**
- **Universal** quantum computing

4-qubit gates

$$e^{-i\Omega \tilde{\sigma}_1^z \tilde{\sigma}_2^z \tilde{\sigma}_3^z \tilde{\sigma}_4^z} =$$

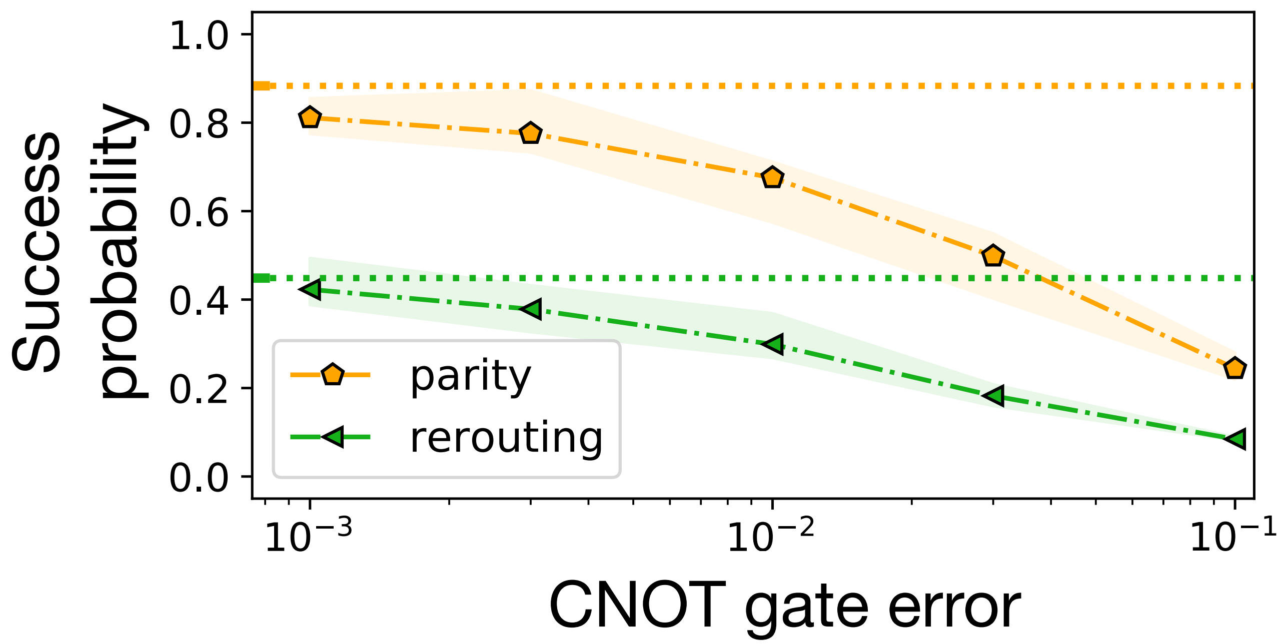


Decoding step: high chance of **measuring invalid states**



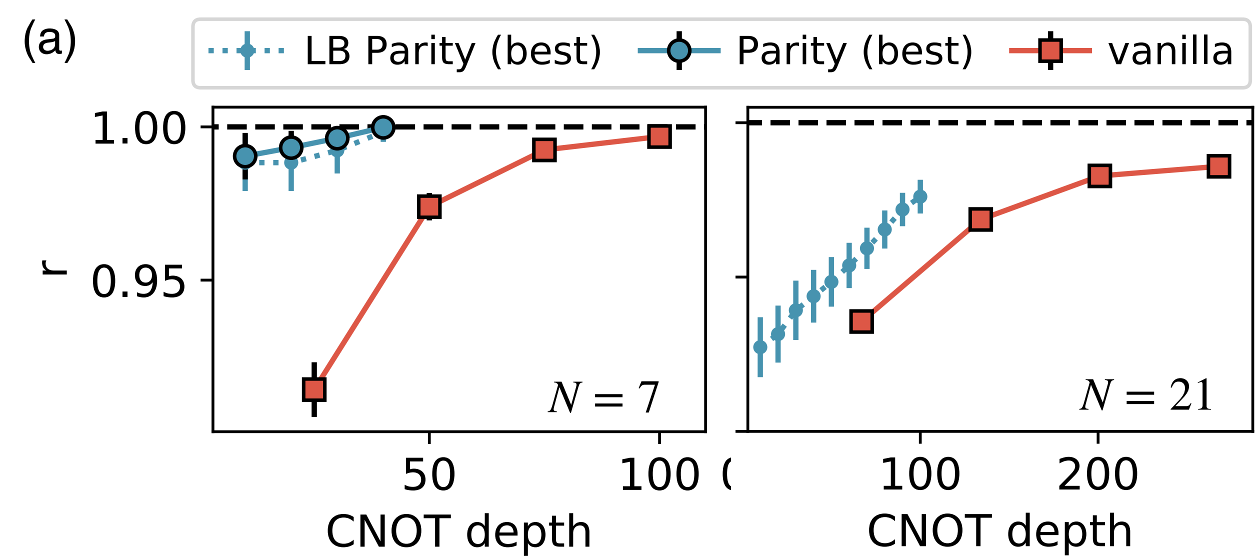
Performance of parity QAOA

[Weidinger, et al PRA 2023]
[Weidinger, et al arXiv 2024]



- $n_l = 6$ classical variables
- $m = 6$ spanning trees
- **Imperfect quantum gates**
- $n_p/n_l = 2.5$ copies for rerouting

- Search is restricted to Clifford circuits
- Computable lower bound on perfromance



Gate sequence

$$\tilde{H}_p = \tilde{H}_z + \tilde{H}_c$$

$$U_z(\gamma) = \mathrm{e}^{-i\gamma \tilde{H}_z}$$

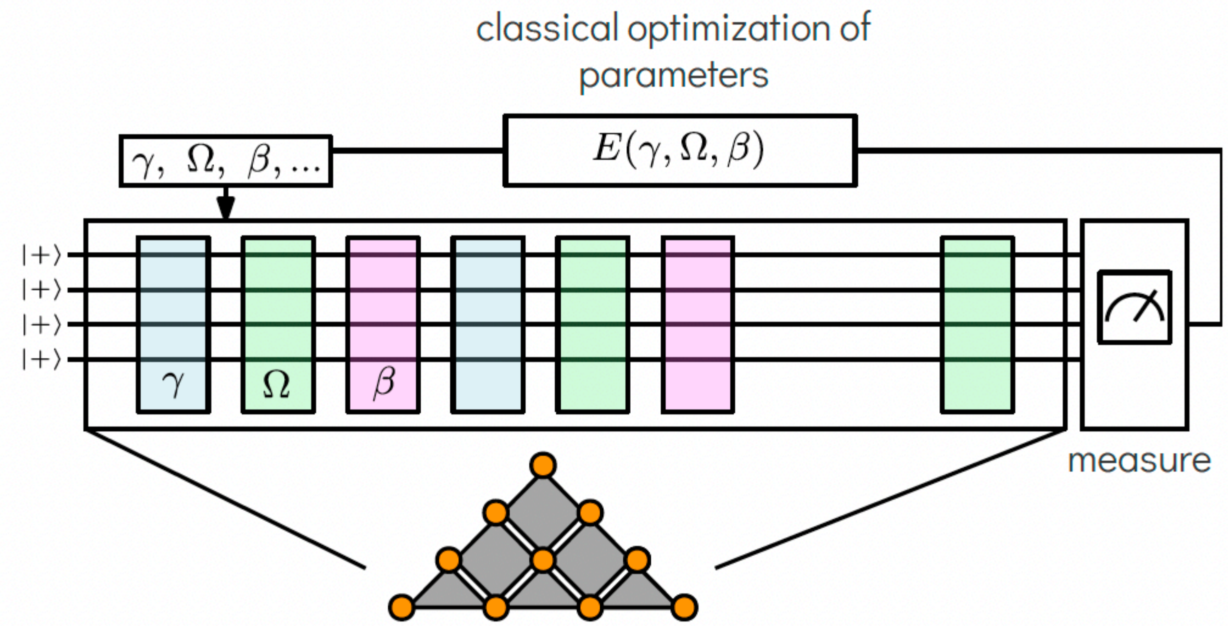
$\hat{\mathrm{Z}}$

$$U_c(\Omega) = \mathrm{e}^{-i\gamma \tilde{H}_c}$$

$\hat{\mathrm{C}}$

$$U_x(\beta) = \mathrm{e}^{-i\beta \tilde{H}_x}$$

$\hat{\mathrm{X}}$



$$A_\lambda^{(l)} = i \sum_{k=1}^{l} \alpha_k \underbrace{[H_a, [H_a, \ldots [H_a,}_{2k-1} \partial_\lambda H_a]]]$$

$$\hat{\mathrm{X}} : \tilde{U}_x(\beta) = \mathrm{e}^{-i\beta \tilde{H}_x}$$

$$\hat{\mathrm{Z}} : \tilde{U}_z(\gamma) = \mathrm{e}^{-i\gamma \tilde{H}_z}$$

$$\hat{\mathrm{C}} : \tilde{U}_c(\Omega) = \mathrm{e}^{-i\Omega \tilde{H}_c}$$

$$\hat{\mathrm{U}}_1 : \tilde{U}_1(\alpha_1) = \mathrm{e}^{-\alpha_1 [\tilde{H}_x, \tilde{H}_z]}$$

$$\hat{\mathrm{U}}_2 : \tilde{U}_2(\alpha_2) = \mathrm{e}^{-\alpha_2 [\tilde{H}_x, \tilde{H}_c]}$$

$$\hat{\mathrm{U}}_3 : \tilde{U}_3(\alpha_3) = \mathrm{e}^{-\alpha_3 [\tilde{H}_x, [\tilde{H}_x, [\tilde{H}_x, \tilde{H}_c]]]}$$

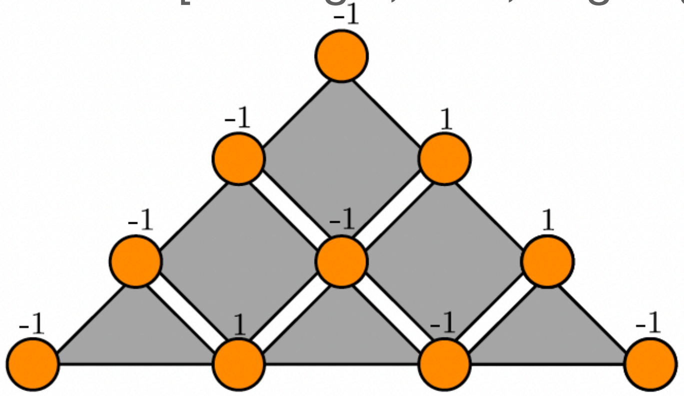
What is the optimal gate sequence?

RL for gate sequences

[Haslinger, et al, ongoing work]

Problem configuration:

- 10 parity qubits
- Local fields $\tilde{J}_i \in \{-1, 1\}$



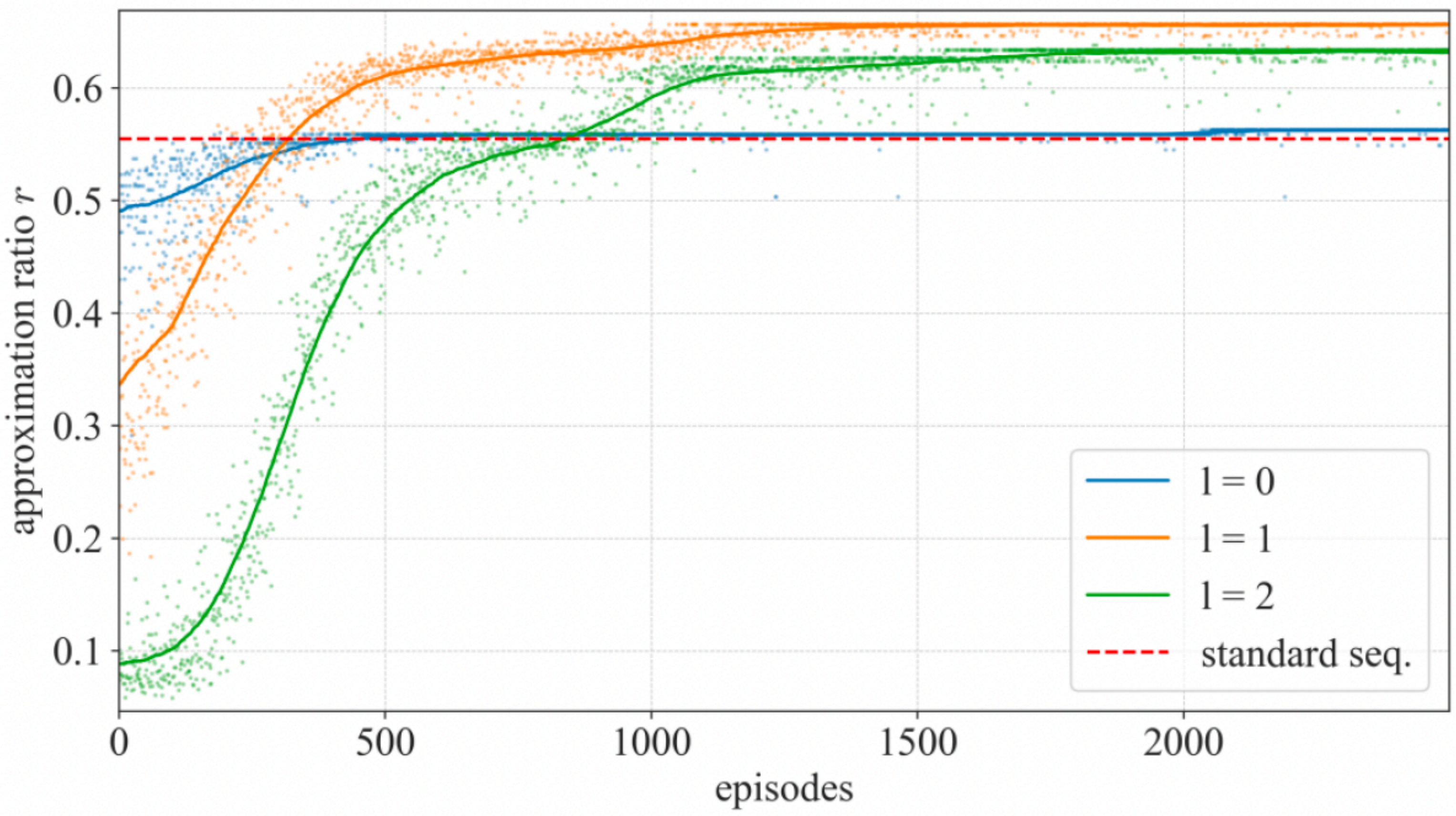
- Learning curves averaged over 10 agents for three gate pools

l = 0: $\{\hat{X}, \hat{Z}, \hat{C}\}$

l = 1: $\{\hat{X}, \hat{Z}, \hat{C}, \hat{U}_1, \hat{U}_2\}$

l = 2: $\{\hat{X}, \hat{Z}, \hat{C}, \hat{U}_1, \hat{U}_2, \hat{U}_3, \hat{U}_4, \hat{U}_5, \hat{U}_6, \hat{U}_7\}$

- Max. gate length $q = 6$
- Energy of discovered sequence is stored



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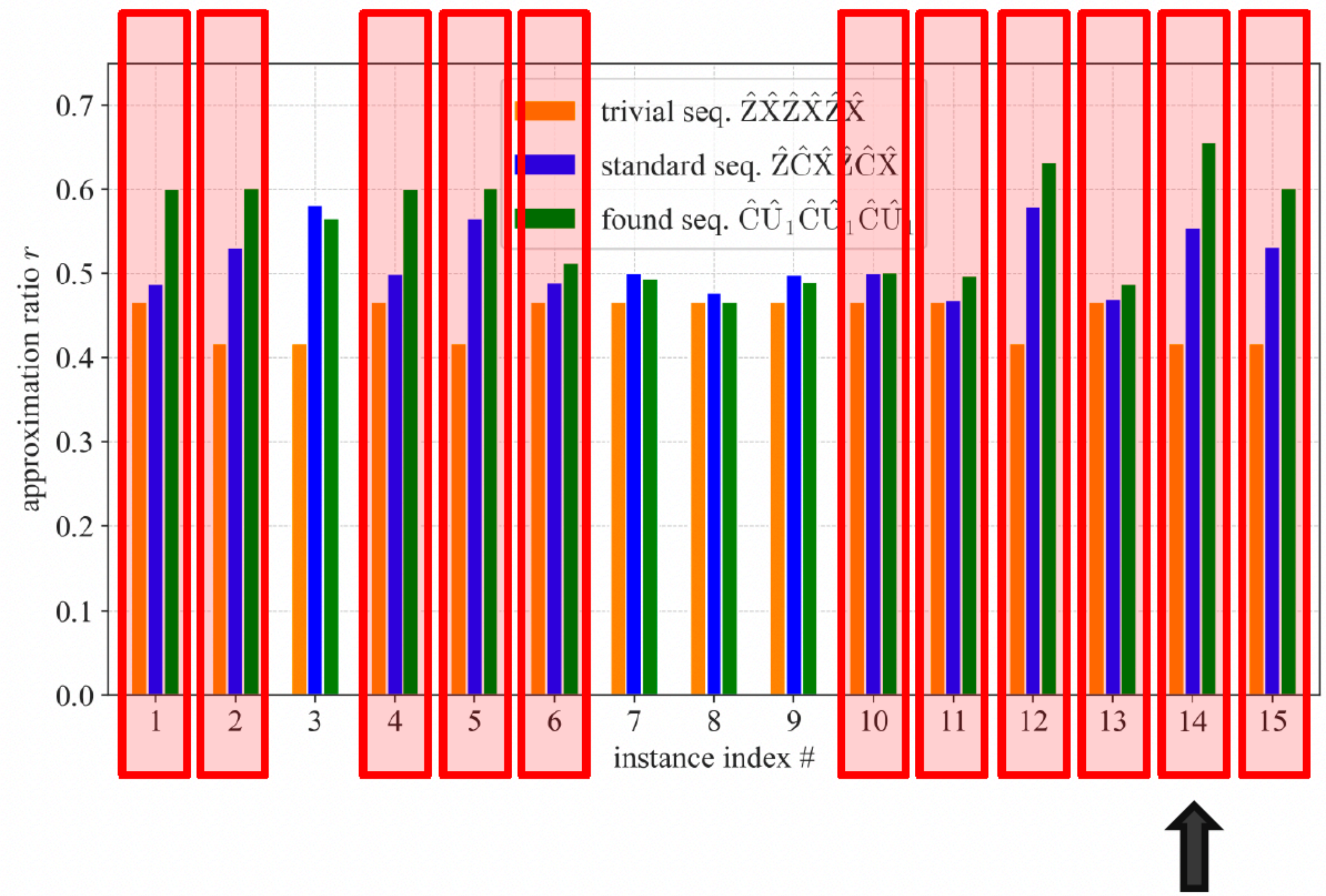
Performace across different istances

- 15 hard problem instances
- 100 random QAOA initializations

→ Found sequence outperforms standard sequence in 11 out of 15 problem instances



Summary

- The presence of **barren plateaus** hinders the **performance of QAOA**
- The **reinforcement learning** optimization converges to smooth optimal schedules, avoiding barren plateaus
- Few observables needed for the learning process
- Optimal gates and parameters can be **transferred among different system sizes**