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On prospects and limitations of variational quantum algorithms

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On the PhD thesis supervised by Jacob Biamonte

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Outlook

1. Theoretical background.
2. Variational quantum algorithms.
3. VQE and QAOA.
4. State preparation QAOA.
5. Parameter miscalibration noise.
6. Hardware-inspired zero noise extrapolation.
7. Hardware-native QAOA ansatz.

Background

- Quantum computing is performed by manipulations of the state of real quantum hardware.
- However, the existing devices are quite noisy and support limited number of operations.
- In these restrictions, a new variational model of quantum computing was proposed.

Theoretical background

Language of quantum computing

1. Single qubit basis: $|0\rangle, |1\rangle$.
2. n-qubit basis: $\{|0\rangle, |1\rangle\}^{\otimes n}$.
3. For a bit string $j = j_1 \dots j_n$, $|j\rangle \equiv |j_1\rangle \otimes \cdots \otimes |j_n\rangle \equiv |j_1 \dots j_n\rangle$.
4. Pauli matrices

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \; Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1}$$

   also sometimes referred to as $\sigma^{x,y,z}$ or $\sigma^{1,2,3}$
5. Pauli strings $P_\alpha = \sigma^{\alpha_1} \otimes \cdots \otimes \sigma^{\alpha_n} \equiv \sigma_1^{\alpha_1} \dots \sigma_n^{\alpha_n}$.

For example, $X_2 \equiv 1 \otimes X \otimes 1 \otimes \cdots \otimes 1$.

Language of quantum computing

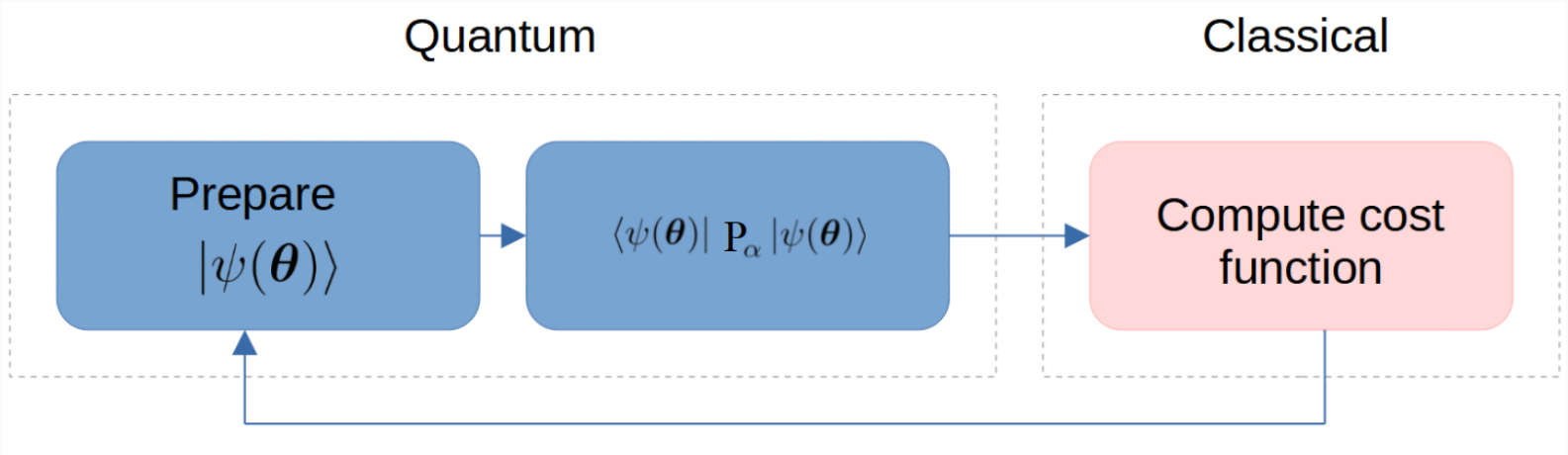
6. Quantum states evolve under unitary operations U (i.e. $U^\dagger = U^{-1}$) as $|\psi_0\rangle \to |\psi\rangle = U|\psi_0\rangle$.
7. Quantum circuits realize unitary operations as a sequence of single and two-qubit gates.
8. Any observable corresponds to a certain hermitian matrix $H = H^\dagger$ and can be decomposed into Pauli strings $H = \sum_\alpha h_\alpha P_\alpha$.

   Expectation value of this observable can be computed by measuring individual Pauli strings as

$$\langle\psi| H |\psi\rangle = \sum_\alpha h_\alpha \langle\psi| P_\alpha |\psi\rangle . \tag{2}$$

Variational Quantum Algorithms

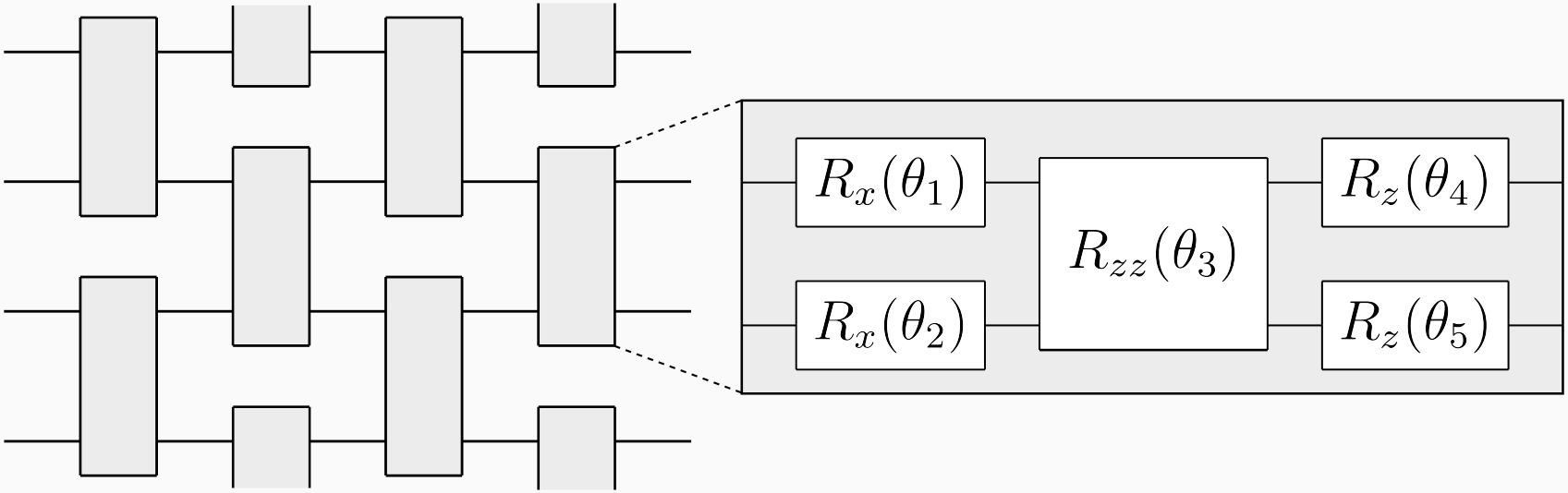
Variational Quantum Algorithms (VQAs)



1. A list of real parameters $\boldsymbol{\theta}$ parametrizes a quantum circuit $U(\boldsymbol{\theta})$.
2. The circuit prepares quantum state $|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})\,|\psi_0\rangle$.
3. A so-called cost function is computed as a sum of expected values of certain observables $E(\boldsymbol{\theta}) = \sum_\alpha h_\alpha \,\langle\psi(\boldsymbol{\theta})|\, P_\alpha\, |\psi(\boldsymbol{\theta})\rangle$.
4. Classical optimization routines update parameters $\boldsymbol{\theta} \to \boldsymbol{\theta}^*$ in an attempt to minimize the cost function.
5. As a result, a certain "desired" state is prepared $|\psi(\boldsymbol{\theta}^*)\rangle = U(\boldsymbol{\theta}^*)\,|\psi_0\rangle$.

Example of variational ansatz

Two layers of checkerboard ansatz for $n = 4$ qubits



$$R_\sigma(\theta) = e^{-i\theta\sigma}$$

$$R_{ZZ}(\theta) = e^{-i\theta Z\otimes Z}$$

Variational Quantum Eigensolvers (VQEs)

VQEs are designed to find ground state $|\psi_g\rangle$ and ground energy E_g of some problem Hamiltonian H. This includes

1. Condensed matter problems: $H = \sum_{neighbours} Z_i Z_j + h \sum_i X_i$.
2. Quantum chemistry problems: $H = \sum_{i,j} h_{ij} c_i^\dagger c_j + \sum_{ijlk} K_{ijlk} c_i^\dagger c_j^\dagger c_l c_k$.
3. Classical optimization problems: $H = \sum_{i,j} W_{ij} Z_i Z_j$.

The cost function $E(\boldsymbol{\theta}) = \langle\psi(\boldsymbol{\theta})| H |\psi(\boldsymbol{\theta})\rangle$ represents the energy to be minimized, following

$$\min_{\boldsymbol{\theta}} \langle\psi(\boldsymbol{\theta})| H |\psi(\boldsymbol{\theta})\rangle \geq \langle\psi_g| H |\psi_g\rangle = \min H. \tag{3}$$

Quantum Approximate Optimization Algorithm (QAOA)

QAOA is a type of VQE, designed to solve combinatorial optimization problems. It uses an ansatz of the form

$$|\psi_p(\boldsymbol{\gamma}, \boldsymbol{\beta})\rangle = \prod_{k=1}^{p} e^{-i\beta_k H_x} \cdot e^{-i\gamma_k H} |+\rangle^{\otimes n}, \tag{4}$$

with two sets of parameters $\boldsymbol{\beta}, \boldsymbol{\gamma}$. Here $H_x = \sum_i X_i$, and $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. The task is to minimize the expectation value of H, by finding

$$\min_{(\boldsymbol{\gamma}, \boldsymbol{\beta})} \langle \psi_p(\boldsymbol{\gamma}, \boldsymbol{\beta})| H |\psi_p(\boldsymbol{\gamma}, \boldsymbol{\beta})\rangle \tag{5}$$

QAOA parameter structure, concentrations and layerwise training saturations

QAOA for state preparation[1]

We use QAOA for the state preparation problem, i.e. $H = \mathbb{1} - |t\rangle\langle t|$:

$$|\psi_p(\boldsymbol{\gamma}, \boldsymbol{\beta})\rangle = \prod_{k=1}^{p} e^{-i\beta_k H_x} \cdot e^{-i\gamma_k |t\rangle\langle t|} \, |+\rangle^{\otimes n} \tag{6}$$

to prepare quantum state $|t\rangle = |\mathbf{0}\rangle \equiv |0\rangle^{\otimes n}$.

Theorem 1

Optimal parameters for depth $p = 1$ QAOA circuit relate as $\gamma = \pi - 2\beta$.

Theorem 2

Optimal parameters for depth $p = 1$ QAOA circuit converge as $\beta n \to \pi$ and $\gamma \to \pi$ when $n \to \infty$.

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[1] **Progress Towards Analytically Optimal Angles in Quantum Approximate Optimization**
D. Rabinovich, R. Sengupta, E. Campos, V. Akshay, and J. Biamonte
Mathematics, 10(15), 2601 (2022)

QAOA for state preparation

We numerically validate that parameters of the last QAOA layer follow the same pattern, $\gamma_p + 2\beta_p = \pi$ as claimed in theorem 1 for up to $p = 5$ layers and $n = 17$ qubits.

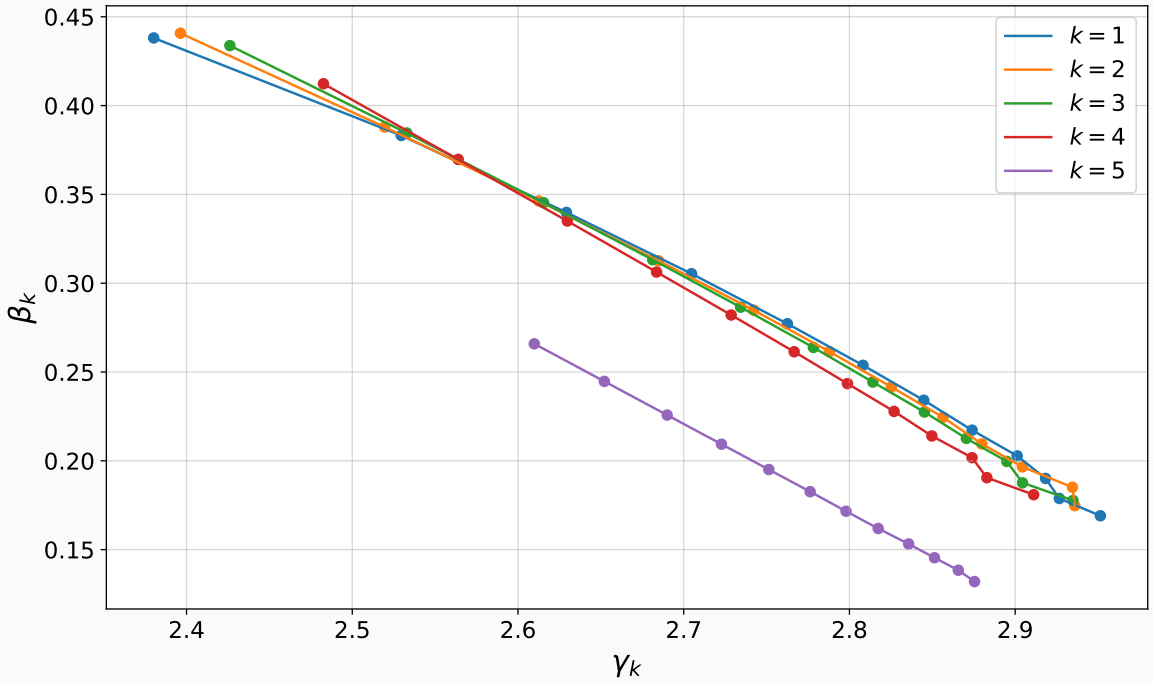


Figure 1: Optimal angles of $p = 5$ depth circuit for $n \in [6; 17]$.

Parameter Concentrations [2]

Definition 1 (Parameter Concentrations)

Given $\boldsymbol{\beta}_n$ and $\boldsymbol{\gamma}_n$, the two p-dimensional vectors of optimal parameters at fixed depth p and n qubits. Then, parameters concentrate whenever

$$\exists\, l > 0 : \forall\, \boldsymbol{\beta}_n, \boldsymbol{\gamma}_n\ \exists\, \boldsymbol{\beta}_{n+1}, \boldsymbol{\gamma}_{n+1} :$$
$$\left|\boldsymbol{\beta}_{n+1} - \boldsymbol{\beta}_n\right|^2 + \left|\boldsymbol{\gamma}_{n+1} - \boldsymbol{\gamma}_n\right|^2 = \mathcal{O}\left(\frac{1}{n^l}\right).$$

[2] Parameter Concentrations in Quantum Approximate Optimization
V. Akshay,D. Rabinovich, E. Campos, J. Biamonte
(Letter) Physical Review A 104, L010401 (2021)

Layerwise QAOA

We again investigate the state preparation QAOA sequence,

$$|\psi_p(\boldsymbol{\gamma}, \boldsymbol{\beta})\rangle = \prod_{k=1}^{p} e^{-i\beta_k H_x} \cdot e^{-i\gamma_k |\mathbf{0}\rangle\langle\mathbf{0}|} \, |+\rangle^{\otimes n} \,, \tag{7}$$

but now optimize its parameters layer by layer, following so called layerwise training strategy.

Definition 2 (Training Saturation)
Training saturates for depth p^*, the smallest depth for which

$$|\langle \mathbf{0}|\psi_{p^*+1}\rangle|^2 \leq |\langle \mathbf{0}|\psi_{p^*}\rangle|^2 \neq 1, \tag{8}$$

Layerwise training saturations[3]

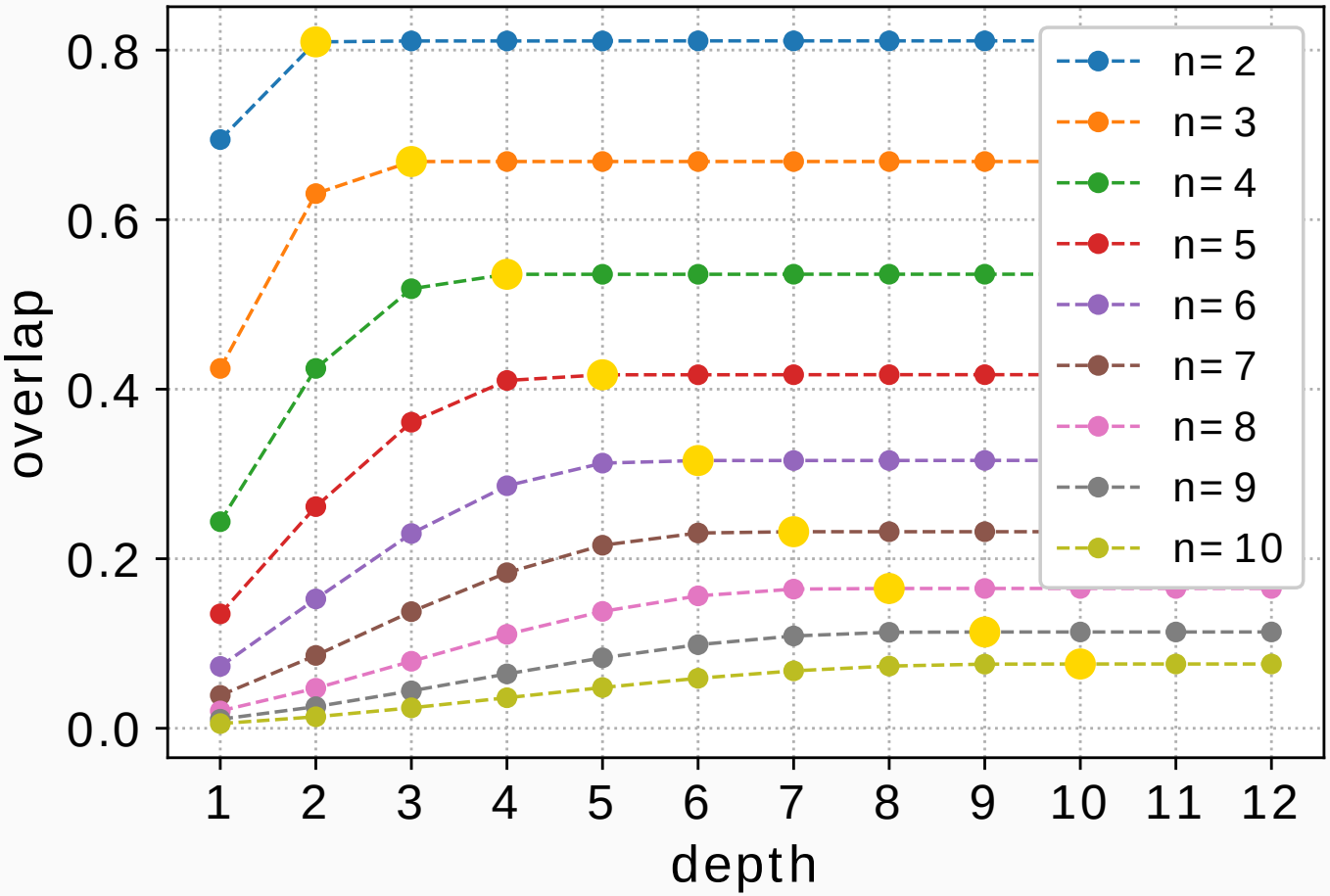


Figure 2: Saturation occurs at $p^* = n$ as indicated by the highlighted points.

[3] Training Saturation in Layerwise Quantum Approximate Optimisation
E.Campos, D.Rabinovich, V.Akshay, J.Biamonte
(Letter) Physical Review A 104, L030401 (2021)

Symmetric subspace

Definition 3 (Dicke vectors)

$$|e_k\rangle = \frac{1}{\sqrt{C_n^k}} \sum_{x_1+\cdots+x_n=k} |x_1 x_2 \ldots x_n\rangle \,, \tag{9}$$

for $k = 0, \ldots, n$.

Any vector from the symmetric subspace can be decomposed over Dicke vectors, $|\psi\rangle = \sum_{k=0}^{n} A_k |e_k\rangle$.

Amplitudes of saturated states

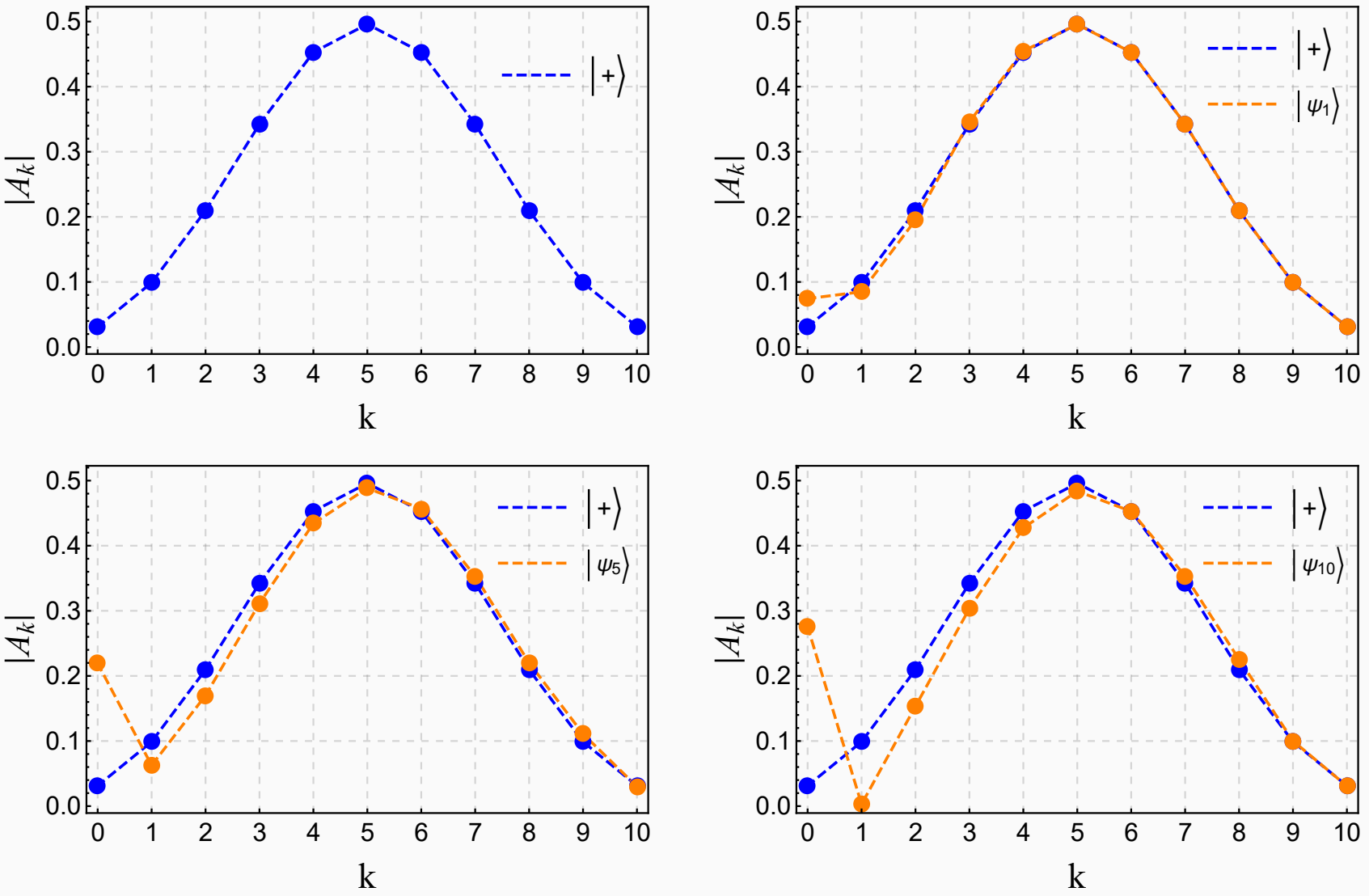


Figure 3: Amplitudes of layerwise optimized QAOA states.

Training saturations

We introduce and prove the necessary saturation conditions:

Proposition 1 (Necessary saturation conditions)

QAOA states $|\psi\rangle = \sum_{k=0}^{n} A_k |e_k\rangle \in H_s$*, whose overlap with the target string* $|\mathbf{0}\rangle$ *can not be increased, using layerwise optimization, satisfy*

$$A_1 \equiv \langle e_1|\psi\rangle = 0, \tag{10}$$

$$|A_2| \equiv |\langle e_2|\psi\rangle| \leq \sqrt{\frac{n}{2(n-1)}} |\langle e_0|\psi\rangle|. \tag{11}$$

Training saturations

Yet, the performance can be improved in the presence of noise. For example, we can miscalibrate parameters slightly after training every layer:

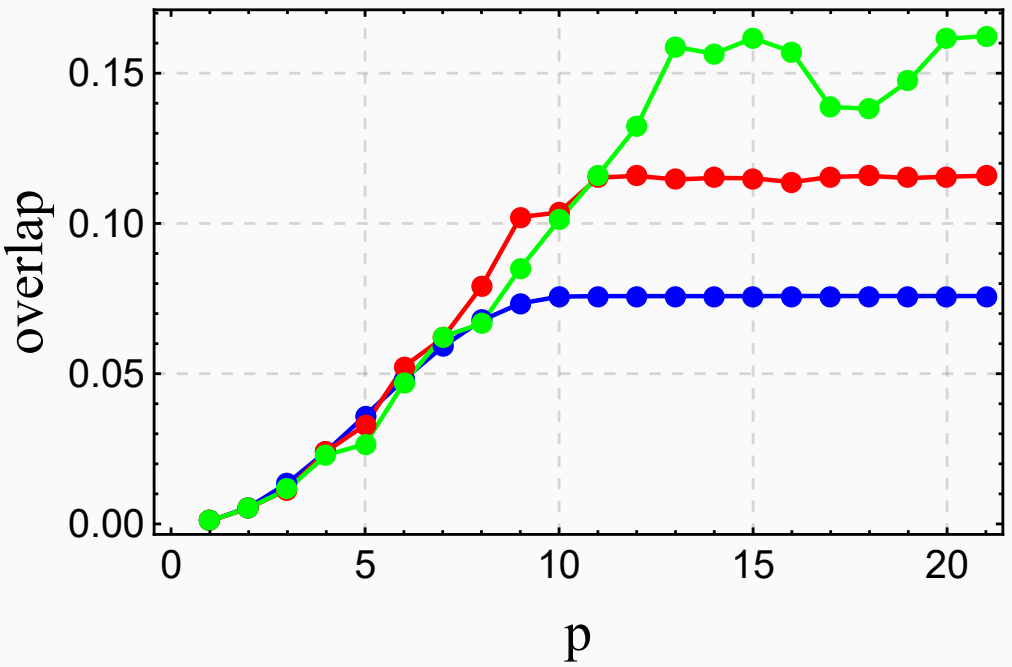


Figure 4: Overlap with respect to circuit depth. (Blue) simple layerwise training, (red) layerwise training with random parameter perturbation from $[-\frac{2\pi}{100}, \frac{2\pi}{100}]$, (green) same but for $[-\frac{3\pi}{100}, \frac{3\pi}{100}]$.

Parameter perturbation noise[4]

[4] **Robustness of variational quantum algorithms against stochastic parameter perturbation**
D. Rabinovich, E. Campos, S. Adhikary, E. Pankovets, D. Vinichenko, J. Biamonte
Physical Review A **109**, 042426 (2024)

Parameter perturbation noise

If we use a parameterized circuit $\prod_{k=1}^{q} U(\theta_k)$ to prepare state $|\psi(\boldsymbol{\theta})\rangle = \prod_{k=1}^{q} U_k(\theta_k)\,|\psi_0\rangle$, due to parameter fluctuation a different state

$$|\psi(\boldsymbol{\theta} + \boldsymbol{\delta\theta})\rangle = \prod_{k=1}^{q} U(\theta_k + \delta\theta_k)\,|\psi_0\rangle\,. \tag{12}$$

ends up being prepared. Importantly, here $\boldsymbol{\delta\theta}$ can vary from experiment to experiment.

Parameter perturbation noise

We describe this form of noise as decoherence

$$|\psi(\boldsymbol{\theta})\rangle\langle\psi(\boldsymbol{\theta})| \rightarrow \rho(\boldsymbol{\theta}) = \int_{\boldsymbol{\delta\theta}\in[-\pi,\pi]^{\times q}} p(\boldsymbol{\delta\theta})\, |\psi(\boldsymbol{\theta}+\boldsymbol{\delta\theta})\rangle\langle\psi(\boldsymbol{\theta}+\boldsymbol{\delta\theta})|\, d(\boldsymbol{\delta\theta}), \tag{13}$$

with $p(\boldsymbol{\delta\theta})$ being the probability density of $\boldsymbol{\delta\theta}$. Any expectation value should now be calculated as $\langle O\rangle(\boldsymbol{\theta}) = Tr(O\rho(\boldsymbol{\theta}))$.

Sensitivity to noise

Theorem 3

Consider a quantum circuit $|\psi(\boldsymbol{\theta})\rangle = U_1(\theta_1)\ldots U_q(\theta_q)\,|\psi_0\rangle$, *where each* $U_k(\theta_k) = e^{iA_k\theta_k}, A_k^2 = \mathbb{1}$. *Assume that every parameter* θ_k *receives a perturbation* $\delta\theta_k$, *sampled from the probability distribution* $p(\delta\theta_k)$. *Assume that (a) perturbations to all the angles are independent, (b) the distribution is symmetric around zero,* $p(\delta\theta) = p(-\delta\theta)$ *and (c) the distribution* $p(\delta\theta_k)$ *vanishes quickly outside a small range* $(-\sigma_k, \sigma_k)$. *Assuming typical strength of the noise to be uniform* $\sigma_k = \sigma$, *under the noise model* (13) *expectation value of any observable* O *changes as*

$$\mathrm{Tr}(\rho(\boldsymbol{\theta})O) - \langle\psi(\boldsymbol{\theta})|\,O\,|\psi(\boldsymbol{\theta})\rangle \propto \sigma^2 \tag{14}$$

in the lowest order in σ.

Sensitivity to noise

For the proof we demonstrate that $\rho(\boldsymbol{\theta}) = |\psi(\boldsymbol{\theta})\rangle\langle\psi(\boldsymbol{\theta})| + \delta\rho$, where

$$\delta\rho \approx -\sum_{k=1}^{q} a_k \, |\psi(\boldsymbol{\theta})\rangle\langle\psi(\boldsymbol{\theta})| + \sum_{k=1}^{q} a_k \, |\psi_k\rangle\langle\psi_k| + O(\sigma_k^4). \tag{15}$$

Here

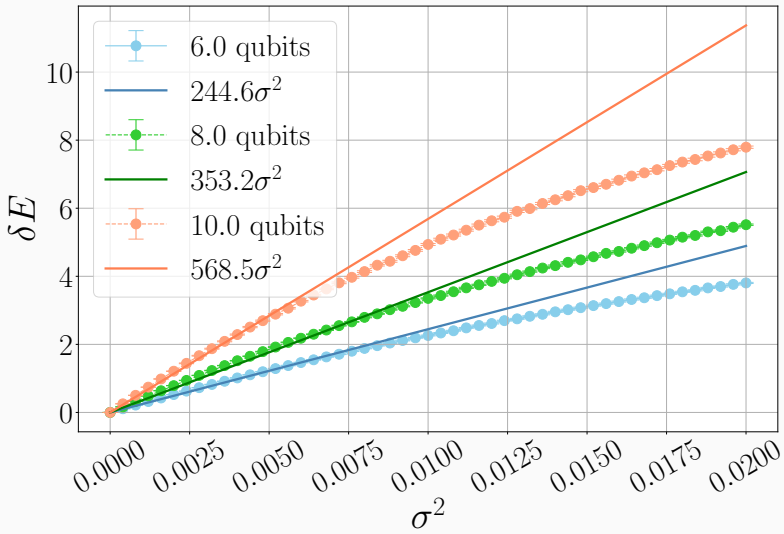
$$a_k \equiv \langle \sin^2 \delta\theta_k \rangle \approx \langle \delta\theta_k^2 \rangle = \int (\delta\theta_k)^2 p(\delta\theta_k) d(\delta\theta_k) \sim \sigma_k^2, \tag{16}$$

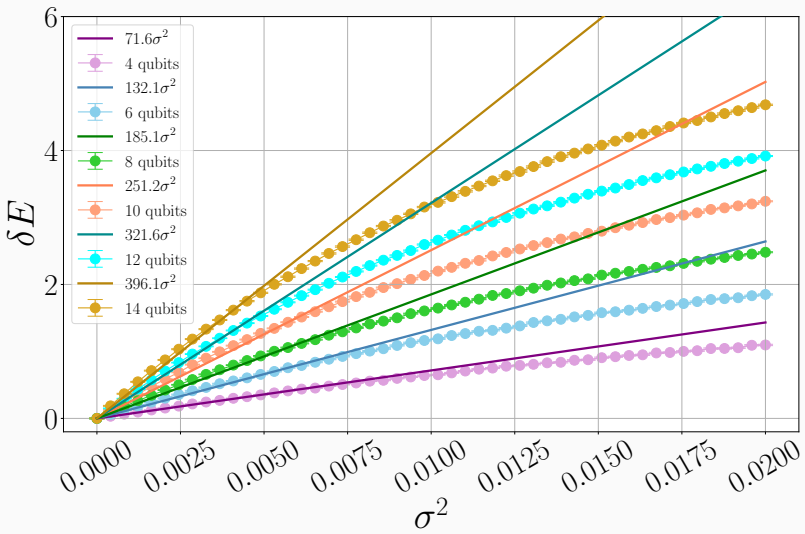
and

$$|\psi_k\rangle = U_1(\theta_1) \ldots U_k\left(\theta_k + \frac{\pi}{2}\right) \ldots U_q(\theta_q) \, |\psi_0\rangle \, . \tag{17}$$

Robustness of VQE

Following examples of VQE, we demonstrate that due to parameter perturbation the energy changes at most as $\delta E \leq q\sigma^2(E_m - E)$, where E_m is the highest eigenvalue of H.





The predicted quadratic scaling appears to prevail all the way up to $q\sigma^2 \lesssim 1$.

Hardware inspired Zero Noise Extrapolation[5]

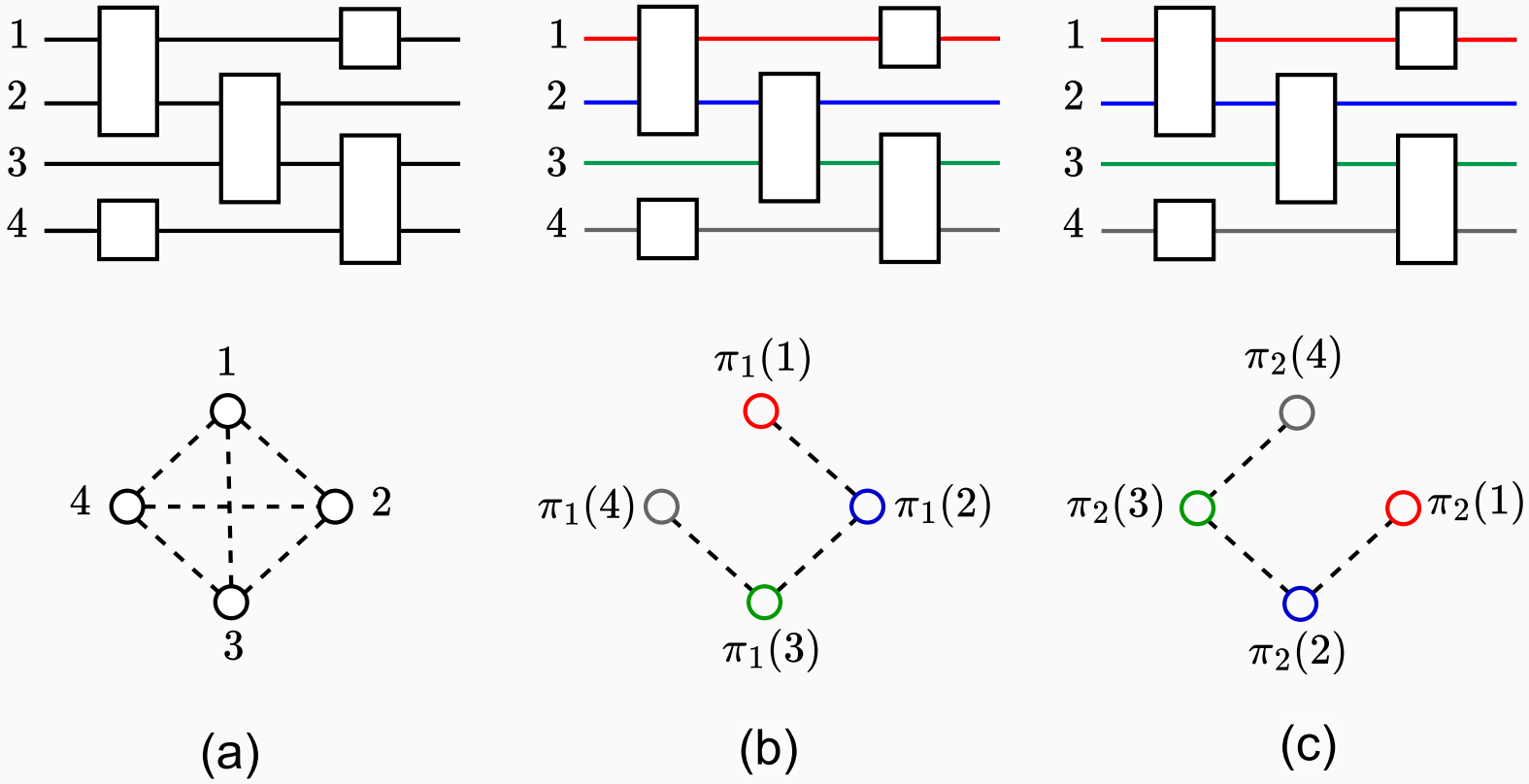
[5] **Mitigating quantum gate errors for variational eigensolvers using hardware-inspired zero-noise extrapolation**
A. Uvarov, D. Rabinovich, O. Lakhmanskaya, K. Lakhmanskiy, J. Biamonte, and S. Adhikary
Physical Review A **110**, 012404 (2024)

Zero Noise Extrapolation

1. In the presence of noise, expectation values of any observable $\langle O \rangle(\lambda)$ become dependent on the strength of the noise λ.
2. Given some control over λ, one can gather statistics for different noise strength.
3. Performing extrapolation $\lim_{\lambda \to 0} \langle O \rangle(\lambda)$, one recovers an approximation to the noiseless expectation value.

Utilizing inhomogeneous error distribution

Due to inhomogeneity of the errors in current devices, different abstract-to-physical qubit mappings naturally give rise to different strength of the noise.



Hardware inspired Zero Noise Extrapolation

We assume that every gate is followed by a noisy channel

$$\Phi_{ij}[\rho] = (1 - q_{\pi(ij)})\rho + q_{\pi(ij)}\mathcal{E}(\rho), \tag{18}$$

whose strength $q_{\pi(ij)}$ depends on the permutation π.

Hardware inspired Zero Noise Extrapolation

In the presence of the noise the energy becomes

$$E = E_0 + \sum_{\substack{(j,k)\in T \\ l\in[1,d]}} q_{\pi(jk)}(E^l_{jk} - E_0) + O(q^2)$$
$$= E_0 + (A - E_0) \sum_{\substack{(j,k)\in T \\ l\in[1,d]}} q_{\pi(jk)} + \sum_{\substack{(j,k)\in T \\ l\in[1,d]}} q_{\pi(jk)}\epsilon^l_{jk} + O(q^2). \quad (19)$$

Here $E_0 = \mathrm{Tr}\,\rho_0 H$, while E^l_{jk} are the energies obtained by applying an error channel $\mathcal{E}$ to qubits (j,k) in the l-th layer of the ansatz.
$A = \frac{1}{|T|d}\sum E^l_{jk}$, $\epsilon^l_{jk} = E^l_{jk} - A$.

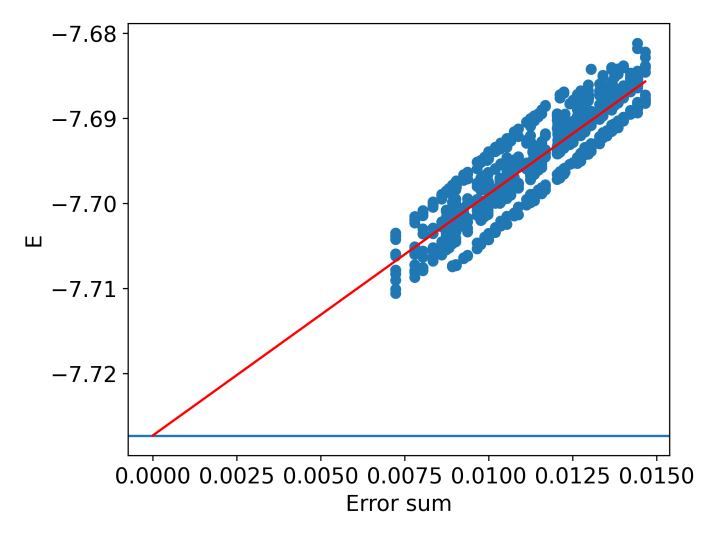
Hardware inspired Zero Noise Extrapolation

Theorem 4

When all qubit permutations $\pi \in S_n$ are considered[6] *and the quantum circuit has a regular multigraph topology, Zero Noise Extrapolation using the permutation fit allows to extrapolate to perfect noiseless expectation value E_0 up to the terms $O(q^2)$.*

[6] The required number of permutations can be reduced from $n!$ to just 2n.

Hardware inspired Zero Noise Extrapolation



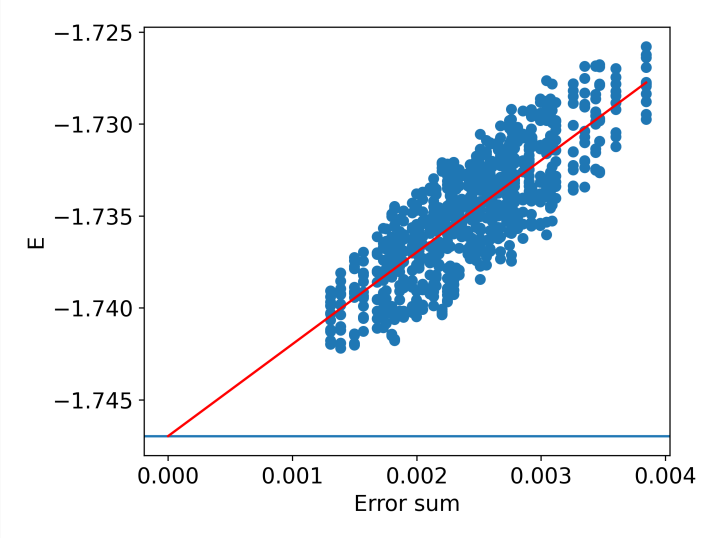


Figure 5: Plots showing Zero Noise Extrapolation using our proposed method for $n = 6$ qubits when all permutations are considered. Ising Hamiltonian (left) and H_2O Hamiltonian (right).

Number of permutations

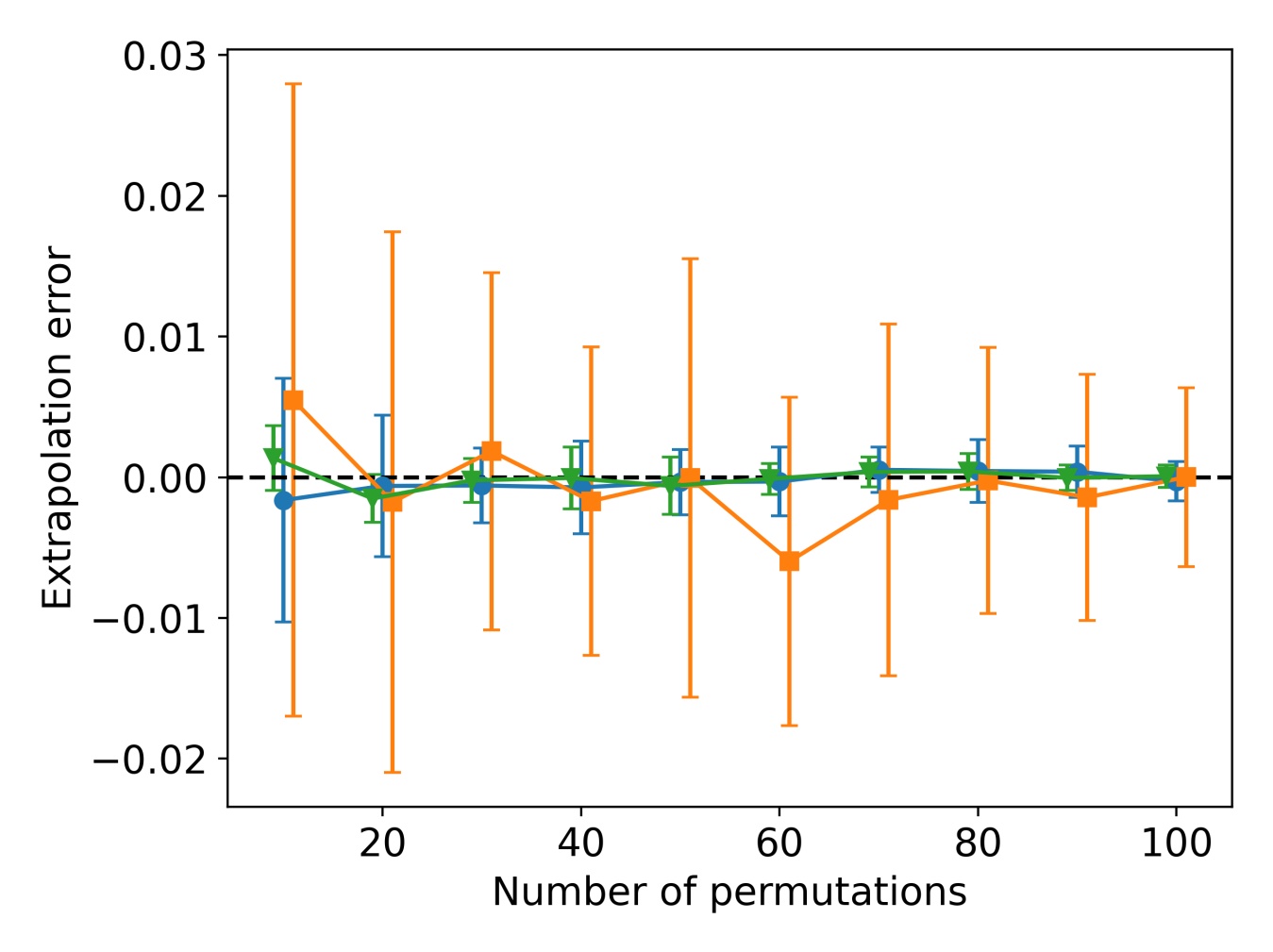


Figure 6: ZNE error versus the number of permutations used.

Strength of the noise

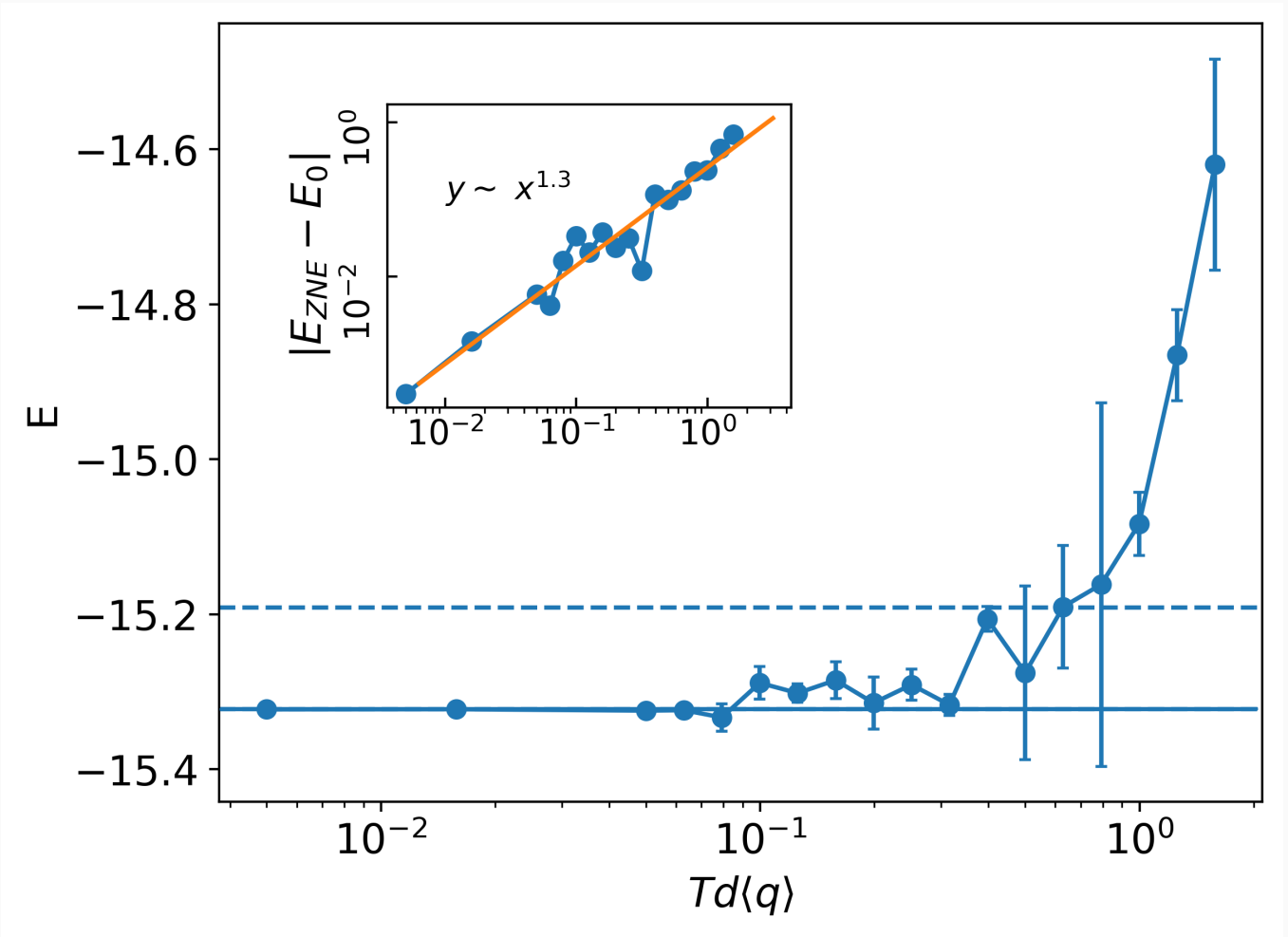


Figure 7: ZNE estimated energy as a function of the magnitude of circuit errors for $n = 12$ qubits.

Hardware native QAOA ansatz[7]

[7] Ion native variational ansatz for quantum approximate optimization
D. Rabinovich, S. Adhikary, E. Campos, V. Akshay, E. Anikin, R. Sengupta, O. Lakhmanskaya, K. Lakhmanskiy, J. Biamonte
Physical Review A 106, 032418 (2022)

QAOA compilation step

Execution of QAOA circuit for some problem Hamiltonian H requires execution of the propagator $\mathbf{exp}\{-i\gamma H\}$, which can be done in two different ways:

1. Native implementation: by letting the system evolve under Hamiltonian H for time γ, naturally inducing the transformation $\mathbf{exp}\{-i\gamma H\}$.
2. Digital implementation: requires a compilation step to decompose the operator $\mathbf{exp}\{-i\gamma H\}$ into a sequence of quantum gates.

Ion native QAOA ansatz

We consider an example of an ion based quantum computer and an ion-native QAOA ansatz

$$|\phi_p(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle = \prod_{k=1}^{p}\left(\exp(-i\beta_k H_x)\exp\left(-i\gamma_k H_I^{ZZ}\right)\right)|+\rangle^{\otimes n}, \tag{20}$$

where

$$H_I^{ZZ} = \frac{J_{\max}}{2}\sum_{j\neq k}\frac{A_j A_k}{|j-k|}Z_j Z_k, \tag{21}$$

and $A_j \in [-1,1]$. The interaction (21) is native to the ion based quantum computers and can be executed naturally, without decomposition into gates.

Ansatz symmetries

The ansatz states are symmetric under bit flip, i.e.

$$X^{\otimes n} |\psi\rangle = |\psi\rangle . \tag{22}$$

Additionally, if $A_j = A_{n-j+1}$, the ansatz possesses additional reflection symmetry $\mathcal{R}$, which acts as $\mathcal{R} |j_1 \dots j_n\rangle = |j_n \dots j_1\rangle$:

$$\mathcal{R} |\psi\rangle = |\psi\rangle . \tag{23}$$

Ion native QAOA ansatz

We use the developed ansatz to solve instances of Sherrington-Kirkpatrick (SK) Hamiltonian

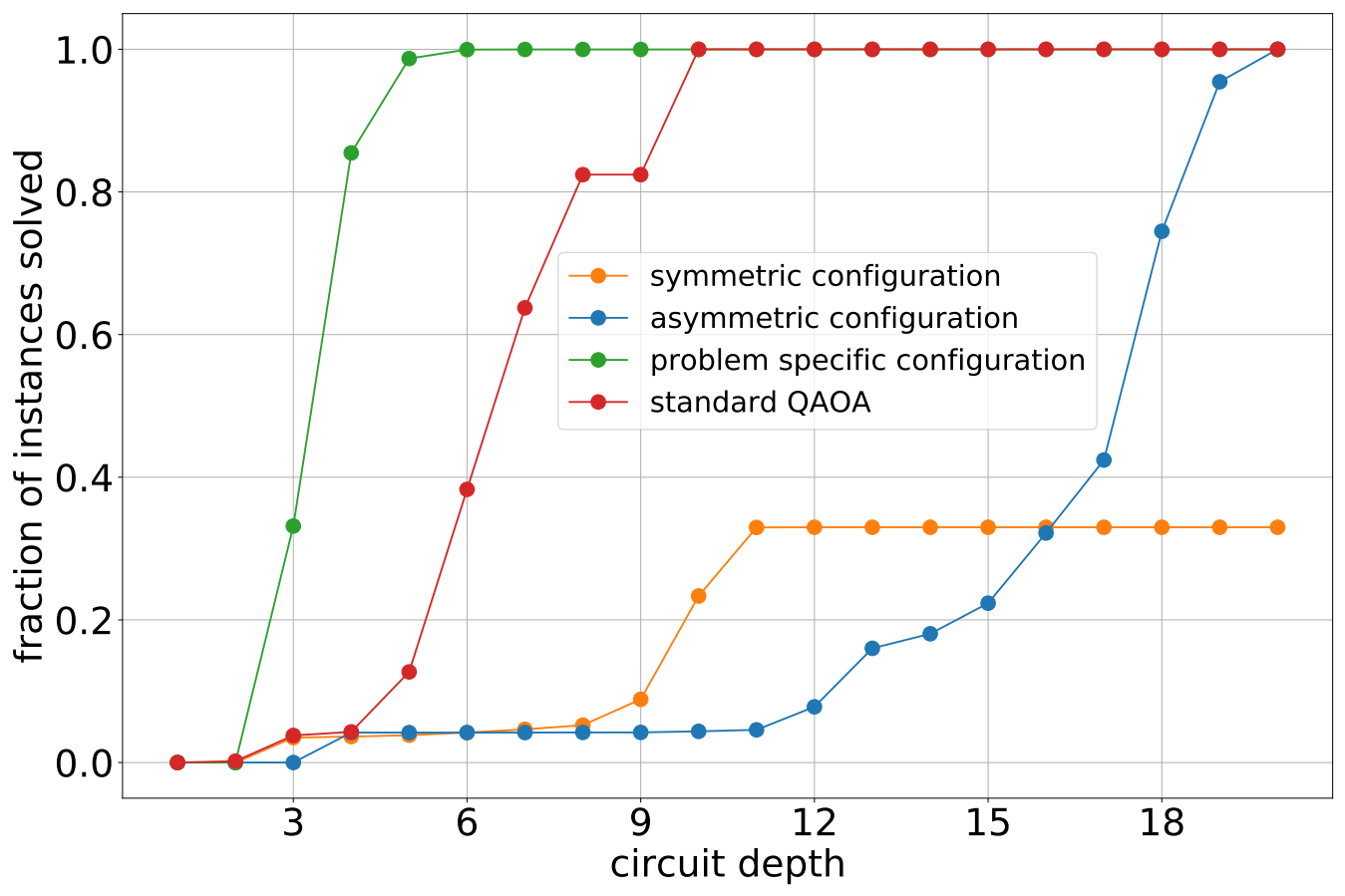
$$H_P = \frac{1}{2} \sum_{j \neq k} K_{jk} Z_j Z_k, \tag{24}$$

$K_{jk} \in [-1, 1]$, which can not be executed natively on the platform. We minimize SK instances with respect to the developed ion native QAOA ansatz (20),

$$\langle \phi_p(\boldsymbol{\gamma}, \boldsymbol{\beta}) | \, H_P \, | \phi_p(\boldsymbol{\gamma}, \boldsymbol{\beta}) \rangle \rightarrow min. \tag{25}$$

Solving SK instances of $n = 6$ qubits

Fraction of SK instances with $n = 6$ that could be minimized by the proposed QAOA ansatz at each depth.



Large system size

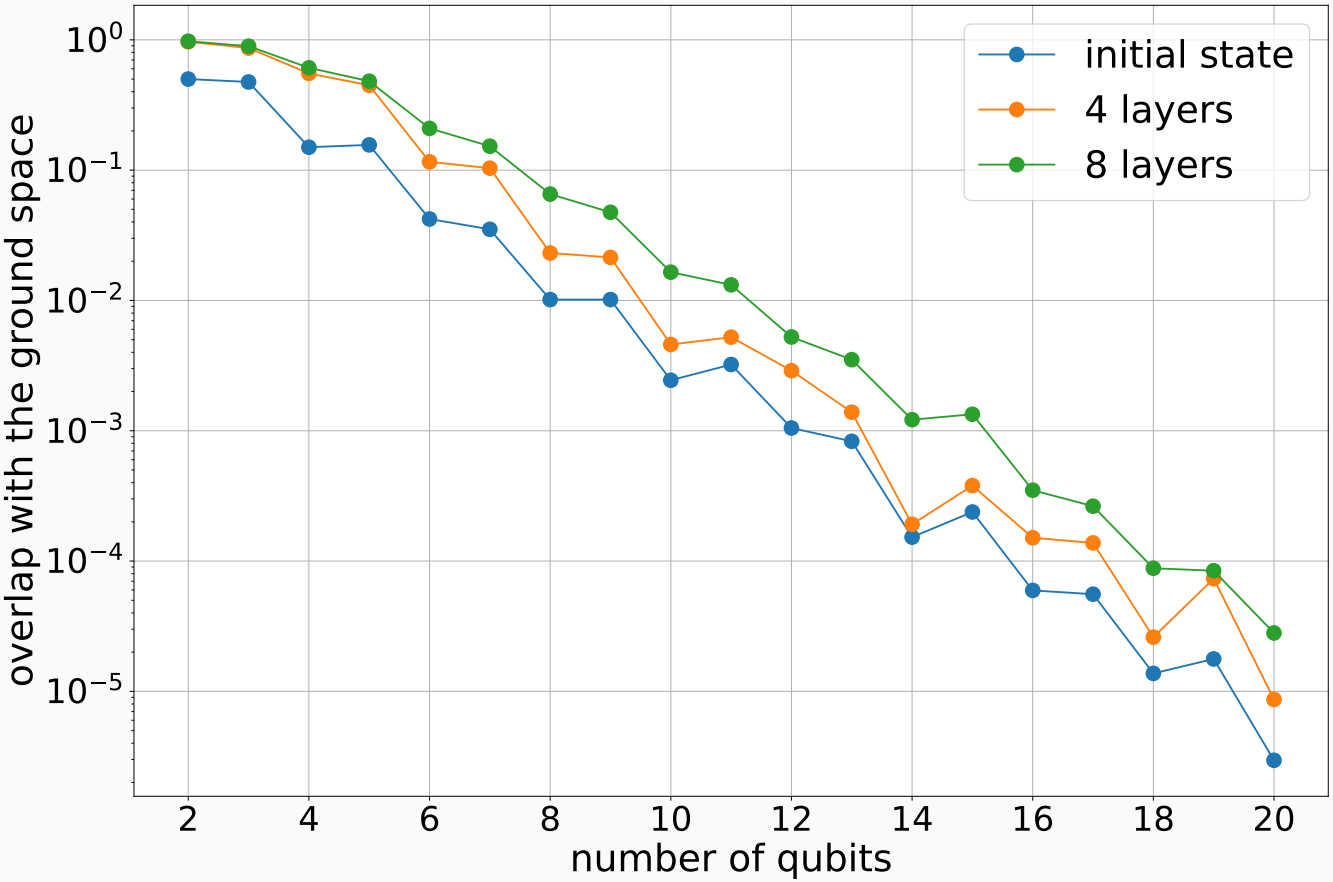


Figure 8: Overlap of the state prepared by the ion native ansatz (20) with the ground space, for different number of qubits and circuit depth.

Conclusions

Conclusions

1. Optimal parameters of state preparation QAOA circuit satisfy (approximately) linear relation.
2. Necessary conditions for the onset of layerwise training saturation were established. Violation of these conditions can remove saturation.
3. In the presence of parameter perturbation noise, expectation values of any observable receive perturbations quadratic in the typical scale of parameter perturbation.
4. A novel Zero Noise Extrapolation strategy, utilizing the inhomogeneity of errors in existing devices, was proposed and tested.
5. A hardware-specific modification of QAOA ansatz was developed and tested.

Thank you for attention!

Appendix

Publication list

Contributing to the thesis

1. E. Campos, **D. Rabinovich**, V. Akshay, J. Biamonte,
   Training Saturation in Layerwise Quantum Approximate Optimisation
   (Letter) Physical Review A **104**, L030401 (2021)
2. **D. Rabinovich**, R. Sengupta, E. Campos, V. Akshay, and J. Biamonte,
   Progress Towards Analytically Optimal Angles in Quantum Approximate Optimisation
   Mathematics, 10(15), 2601 (2022)
3. **D. Rabinovich**, S. Adhikary, E. Campos, V. Akshay, E. Anikin, R. Sengupta, O. Lakhmanskaya, K. Lakhmanskiy, J. Biamonte,
   Ion native variational ansatz for quantum approximate optimization
   Physical Review A 106, 032418 (2022)
4. **D. Rabinovich**, E. Campos, S. Adhikary, E. Pankovets, D. Vinichenko, J. Biamonte,
   Robustness of variational quantum algorithms against stochastic parameter perturbation
   Physical Review A **109**, 042426 (2024)
5. A. Uvarov, **D. Rabinovich**, O. Lakhmanskaya, K. Lakhmanskiy, J. Biamonte, and S. Adhikary
   Mitigating quantum gate errors for variational eigensolvers using hardware-inspired zero-noise extrapolation
   Physical Review A **110**, 012404 (2024)

Publication list

Other works

4. V. Akshay, **D. Rabinovich**, E. Campos, J. Biamonte,
   Parameter Concentrations in Quantum Approximate Optimization
   (Letter) Physical Review A 104, L010401
5. V. Akshay, H. Philathong, E. Campos, **D. Rabinovich**, I. Zacharov, Xiao-Ming Zhang, Dingshun Lv, Man-Hong Yung, J. Biamonte
   Circuit depth scaling for quantum approximate optimization
   Physical Review A 106, 042438 (2022)
6. E. Campos, **D. Rabinovich**, A. Uvarov,
   Depth scaling of unstructured search via quantum approximate optimization
   Physical Review A 110.1 (2024): 012428

Energy vs ground state overlap

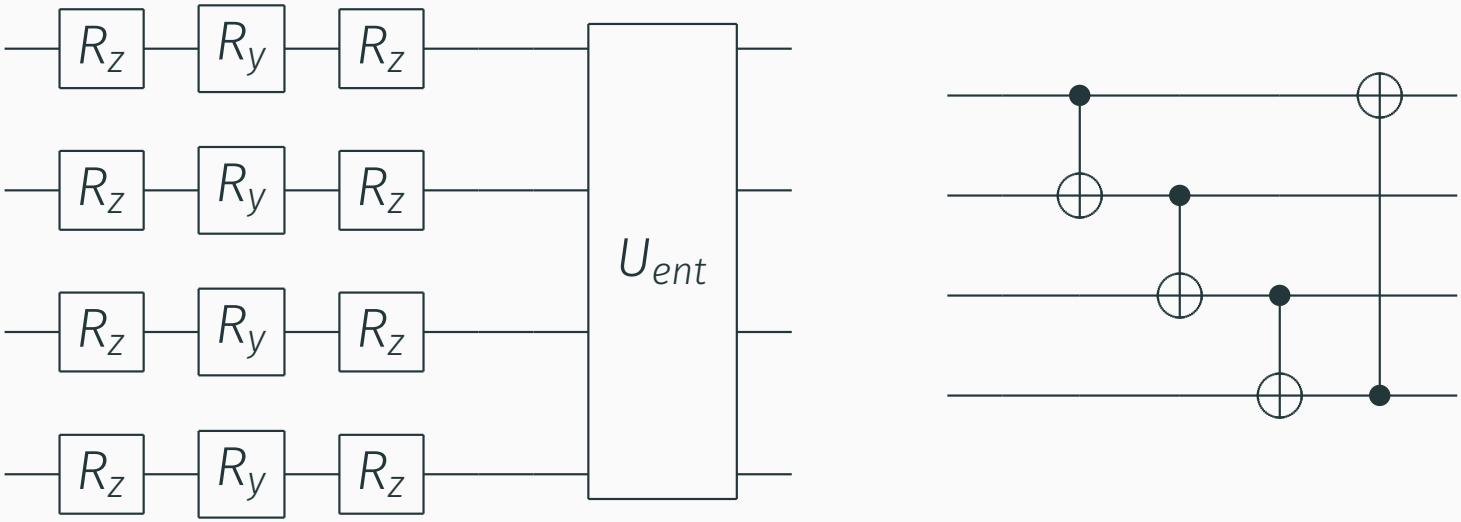
Certain amount of overlap with the ground state can be sufficient to guarantee success. Having prepared a state of overlap g with the ground state, the probability to measure the ground state at least once in k measurements is given by

$$p_k = 1 - (1 - g)^k. \tag{26}$$

For $g = 0.01$, $p_{100} = 0.63$, $p_{500} = 0.99$.

Hardware efficient ansatz

Single layer of the hardware efficient ansatz for $n = 4$ qubits (left) and an example of entangling operator (right)



Example of depth $p = 2$ checkerboard ansatz of $n = 4$ qubits.

Role of the problem Hamiltonian in VQE

In VQE we do not need to simulate the evolution under problem Hamiltonian H, we only need to measure it. For that we

1. Decompose H into a sum of Pauli strings P_α, $H = \sum h_\alpha P_\alpha$.
2. Store the set $\{h_\alpha, P_\alpha\}_\alpha$ on a classical computer.
3. Measure expectation values of Pauli strings P_α on a quantum computer in the state, prepared by the ansatz.
4. Pass the measured values to the classical computer, which computes the energy cost function as

$$\langle \psi(\boldsymbol{\theta}) | H | \psi(\boldsymbol{\theta}) \rangle = \sum_\alpha h_\alpha \langle \psi(\boldsymbol{\theta}) | P_\alpha | \psi(\boldsymbol{\theta}) \rangle . \tag{27}$$

Statement defended

For the QAOA circuit with an n qubit problem Hamiltonian $H = \mathbb{1} - |t\rangle\langle t|$ we

1. Prove a linear relation $\gamma + 2\beta = \pi$ between optimal parameters for $p = 1$ depth circuit of an arbitrary problem size.
2. Numerically validate the linear relation $\gamma + 2\beta = \pi$ between optimal parameters of the last QAOA layer for system sizes up to $n = 17$ qubits and circuit depth $p = 5$.

Statement defended

For QAOA circuit with an n qubit problem Hamiltonian $H = \mathbb{1} - |t\rangle\langle t|$ trained with the layerwise training strategy we

1. Prove the existence of nontrainable quantum states, whose overlap with the target bitstring $|t\rangle$ can not be improved.
2. Formulate and prove necessary conditions for the onset of layerwise training saturation.

Statement defended

Under the weak parameter perturbation assumption, when every parameter of a quantum circuit receives a stochastic perturbation of typical scale σ we prove that the expectation value of any observable is perturbed by a term, proportional to σ^2.

Statement defended

Under the assumption of inhomogeneously distributed errors across the gates between different pairs of qubits a method of Zero Noise Extrapolation is proposed. In this method, the effective strength of the noise is varied by considering different abstract to physical qubit mappings.

1. The method is proven to recover exact noiseless value up to terms, quadratic in the strength of the noise, for circuits of regular graph topology when all qubit permutations are considered.
2. Numerical simulations of the proposed method using only up to 100 permutation allows recovering VQE noiseless energy for transverse field Ising model and water molecule with accuracy of 10^{-2} and better for up to 12 qubits.

Statement defended

QAOA ansatz can be modified to take native system interactions into account, which bypasses the gate based model. For the example of ion based quantum computer, this allowed to modify QAOA to solve arbitrary instances of Sherrington-Kirkpatrick Hamiltonian of $n = 6$ qubits with at most 0.75 energy error using no more than 6 layers of the developed ansatz.