Quantum combinatorial optimization in High-Energy Physics

Yahui Chai

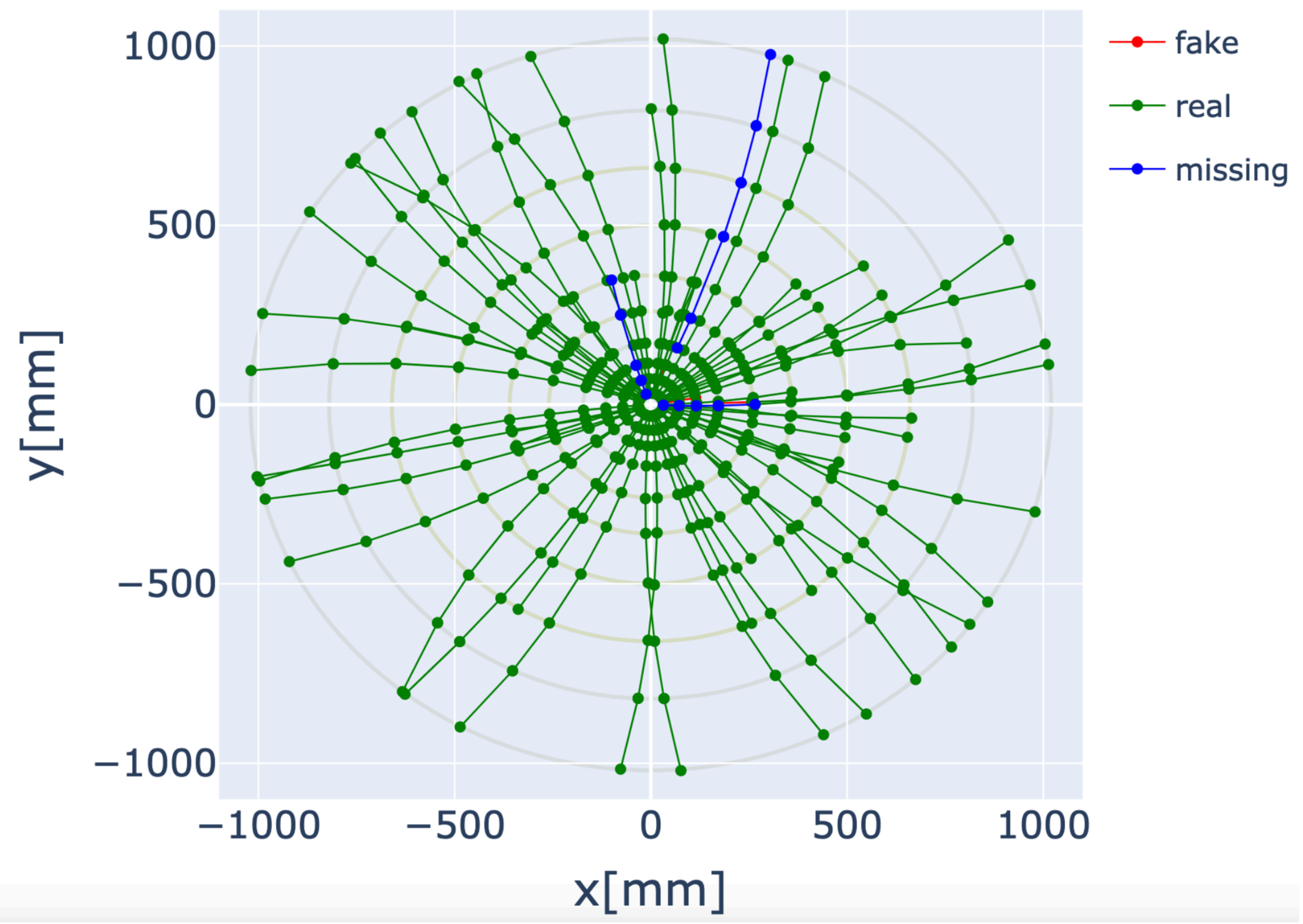
DESY. QUANTUM
Center for Quantum Technology and Applications

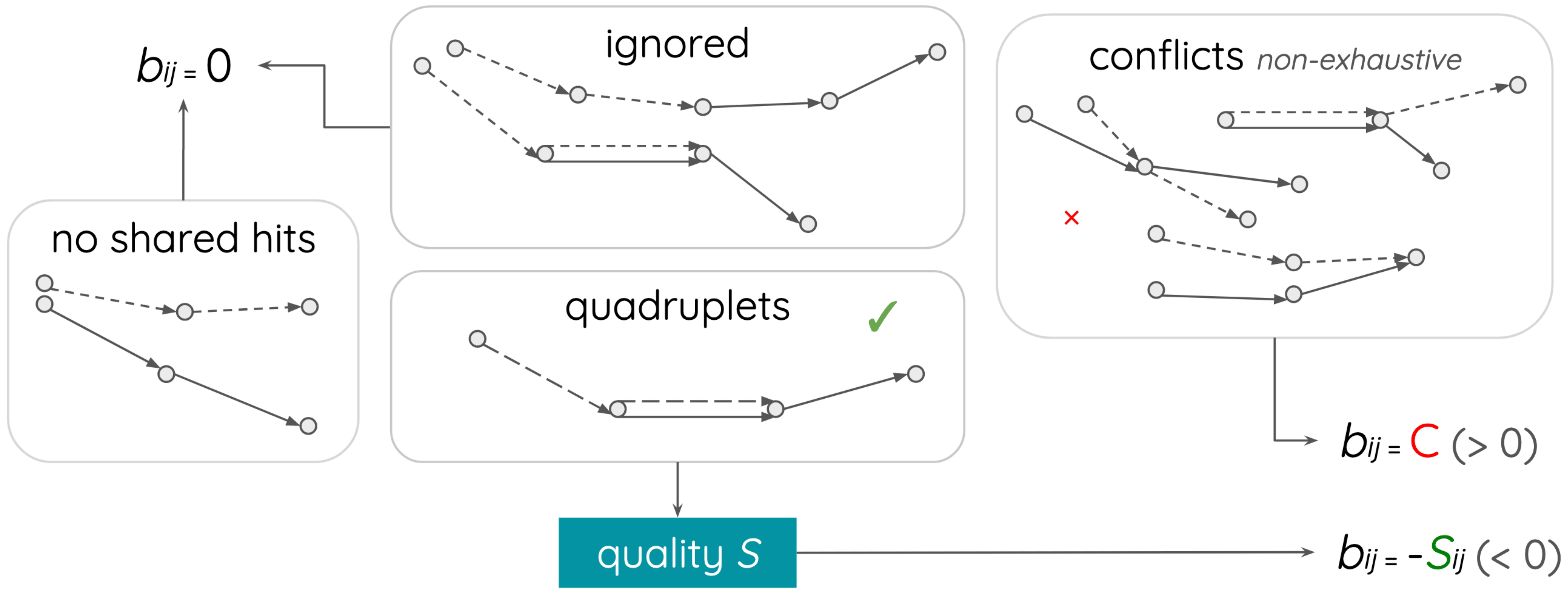
Outline

- An example of Quantum optimization in HEP
  - Particle tracking — Variational Quantum Eigensolver (VQE)
- Development of Quantum optimization problem
  - Structure-inspired ansatz and warm start of VQE
- Short introduce of real-time dynamics of HEP in quantum computing
  - Particle scattering in a fermonic model
  - Meson's Parton distribution functions (PDFs) in Schwinger model
- Summary and outlook

Particle tracking

T. Schwägerl, C. Issever, K. Jansen, T. J. Khoo, S. Kühn, C. Tüysüz, and H. Weber,
Particle Track Reconstruction with Noisy Intermediate-Scale Quantum Computers, arXiv:2303.13249.





- The value assigned to the QUBO quadratic weights b_{ij} for different configurations of the pairs of triplets T_i and T_j

- Hits and reconstructed trajectories of particles in the transverse plane of the detector.

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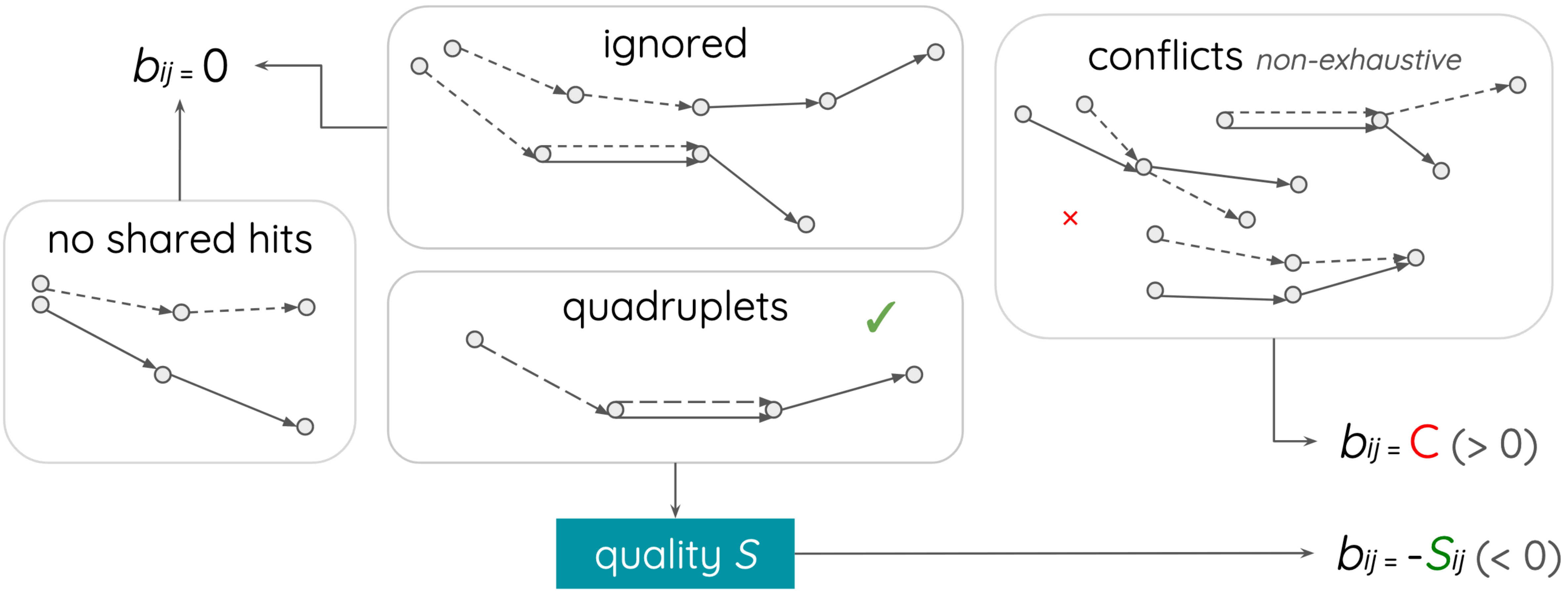
- Construct QUBO cost function

$$Q(T) = \sum_{i}^{N} a_i T_i + \sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j$$

  - Variables: $T_i \begin{cases} 1 & \text{True triplets} \\ 0 & \text{False triplets} \end{cases}$

  - Coefficients: $\begin{cases} a_i & \text{rate the quality of individual triplets} \\ b_{ij} & \text{express the compatibility of two triplets} \end{cases}$



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- Minimize cost function

$$Q(T) = \sum_{i}^{N} a_i T_i + \sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j$$

$$T_i = (I - Z_i)/2$$

$$T_i |0\rangle = 0$$

$$T_i |1\rangle = |1\rangle$$

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- Find the ground state of a Hamiltonian

$$H = \sum_{i}^{N} h_i \cdot Z_i + \sum_{i}^{N} \sum_{j<i}^{N} J_{ij} \cdot Z_i Z_j$$

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Quantum Algorithms

- Get the ground state bit string from measurements

$$e.g., |111000\rangle$$

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Quantum Algorithms

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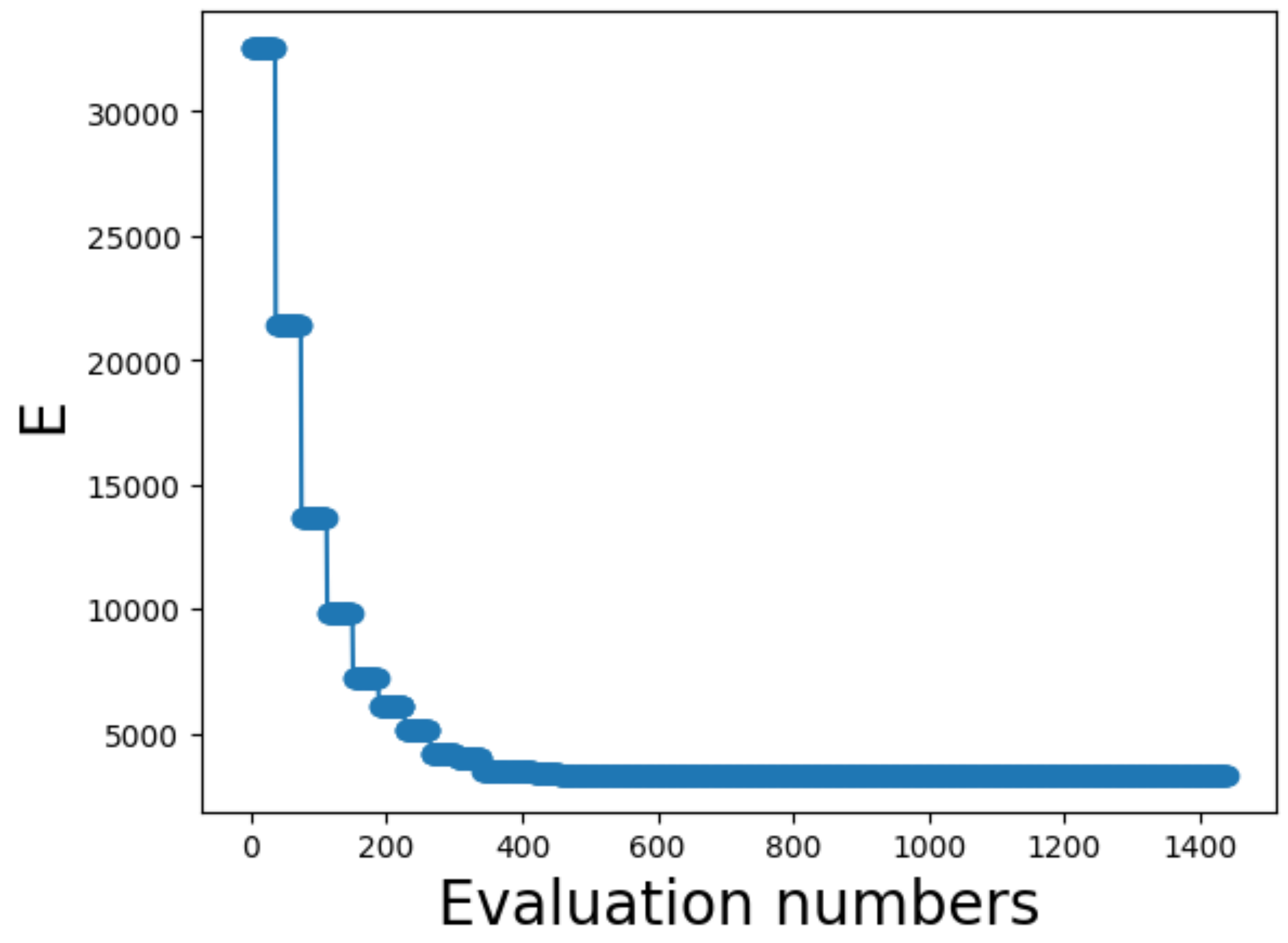
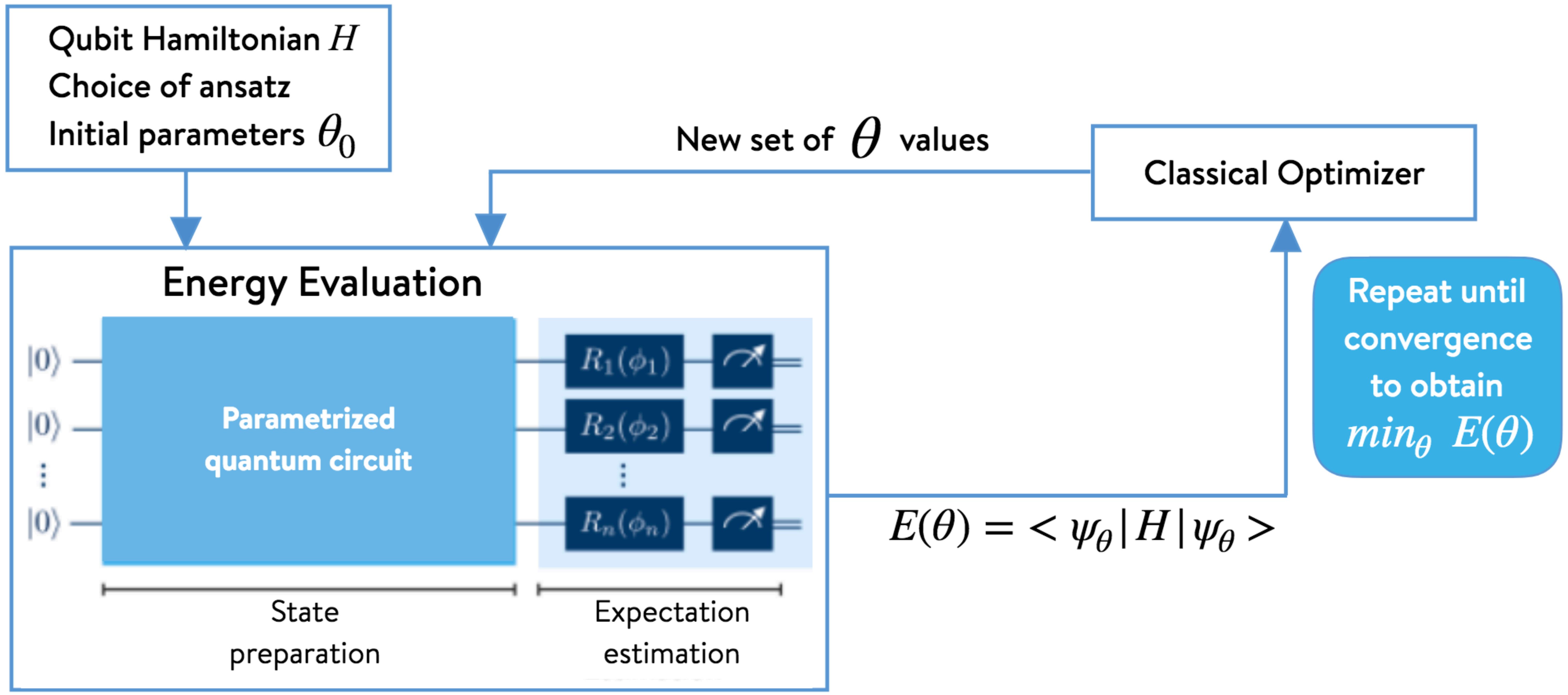
$e.g., |111000\rangle$

- Got the solution

The triplets T_0, T_1, T_2 are true

Variational Quantum Eigensolver (VQE)





http://openqemist.1qbit.com/docs/vqe_microsoft_qsharp.html

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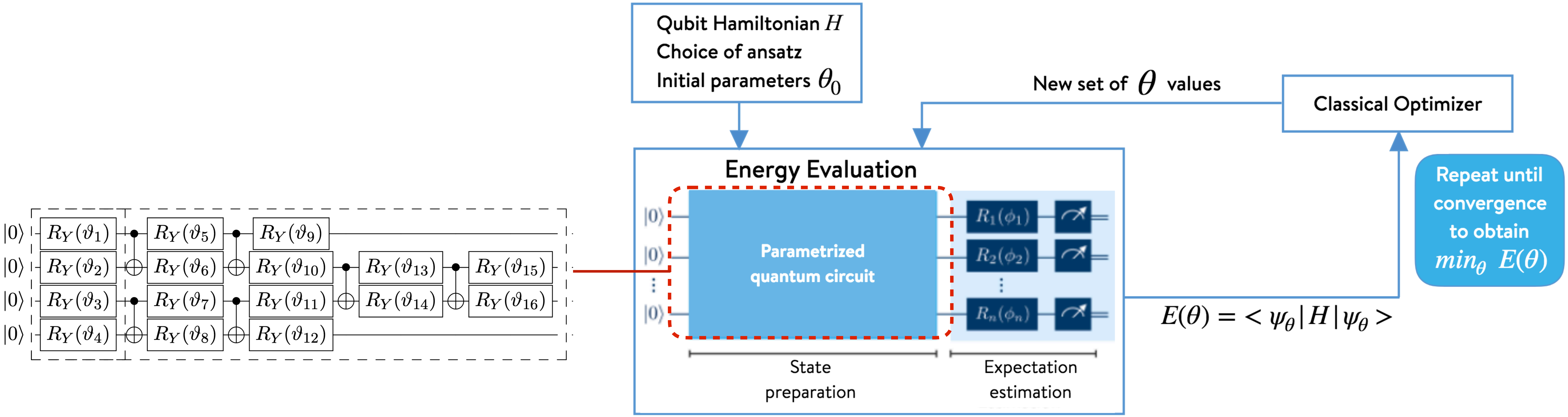

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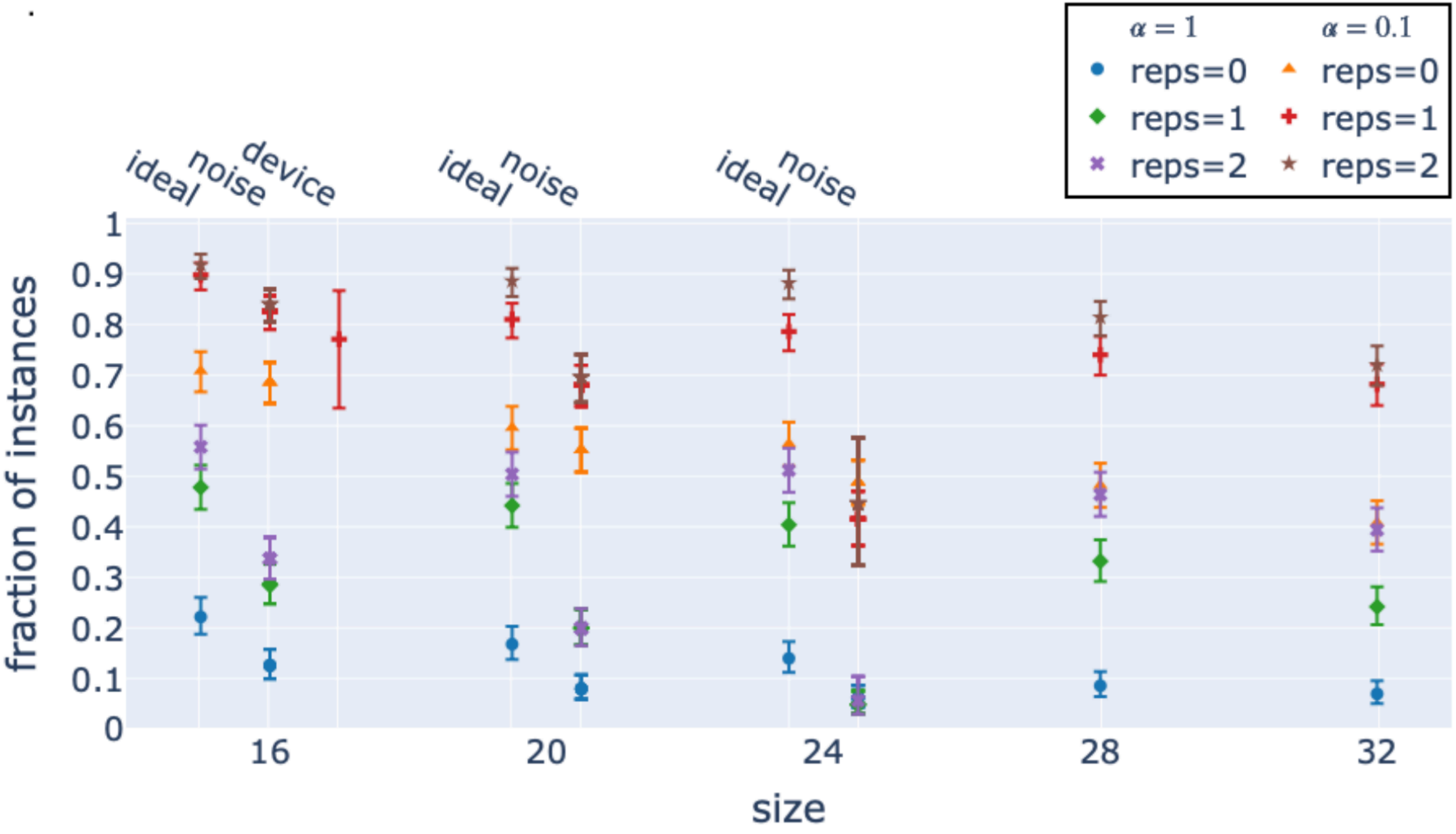
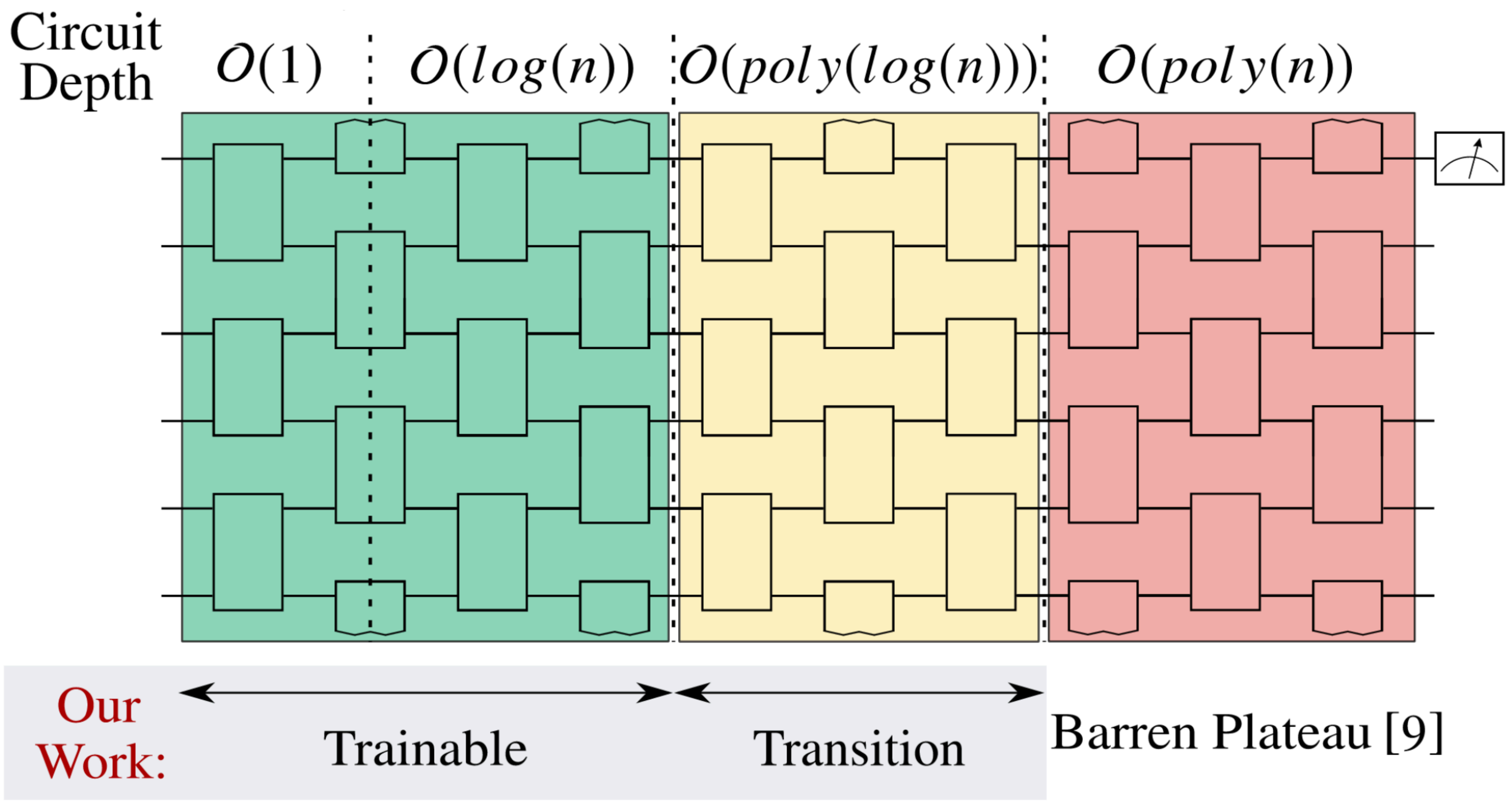
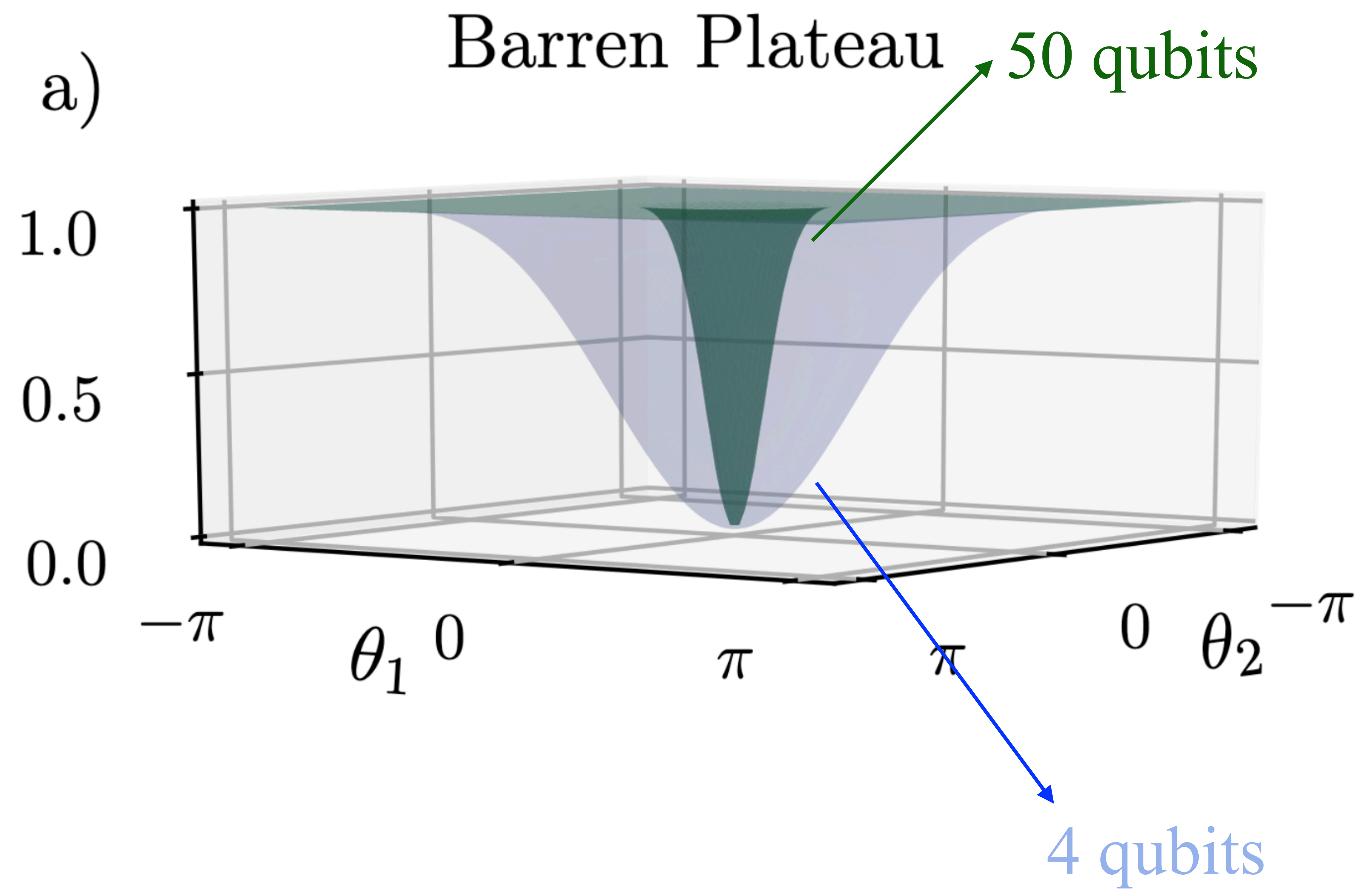
Results via VQE



Challenge in VQE…

- Increasing layers (parameters) for larger system size
  - Might have Barren plateau





[1] M. Cerezo, A. Sone, T. Volkoff, L. Cincio, and P. J. Coles, Cost function dependent barren plateaus in shallow parametrized quantum circuits, Nat Commun 12, 1791 (2021).

[2] A. Arrasmith, Z. Holmes, M. Cerezo, and P. J. Coles, Equivalence of Quantum Barren Plateaus to Cost Concentration and Narrow Gorges.

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How to find a good initial parameter?

A Structure-inspired ansatz for QUBO

- Consider a random QUBO defined on a graph $G(V,E)$:

$$H = \sum_{i \in V} h_i \cdot Z_i + \sum_{(i,j) \in E} J_{ij} \cdot Z_i Z_j, \quad h_i, J_{ij} \in [-1,1]$$

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- The Imaginary time evolution of the QUBO Hamiltonian:

$$e^{-\tau \cdot H} \cdot |+\rangle^{\otimes N} = e^{-\tau \cdot H} \cdot \sum_{k=0}^{2^N-1} a_k |E_k\rangle$$

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Imaginary time evolution (ITE) of QUBO

$$e^{-\tau \cdot H} = e^{-\tau \cdot \left(\sum_i h_i \cdot Z_i + \sum_{(i,j)} J_{ij} \cdot Z_i Z_j \right)}$$

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How to approximate the ITE using a Quantum Circuit?

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Mimic ITE using local quantum gate

Two body term:

ITE: $|\psi_k\rangle = e^{-\tau J_{ij} \cdot Z_i Z_j} |\psi_{k-1}\rangle$

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$$|\psi_k\rangle \sim e^{-i(\alpha_{ij} Z_i Y_j + \beta_{ij} Y_i Z_j)/2} |\psi_{k-1}\rangle$$

Imaginary time evolution (ITE) of QUBO

$$e^{-\tau \cdot H} = e^{-\tau \cdot \left(\sum_i h_i \cdot \sigma_i^z + \sum_{(i,j)} J_{ij} \cdot \sigma_i^z \sigma_j^z \right)}$$
$$= \prod_{(i,j)\in E} e^{-\tau J_{ij} \sigma_i^z \sigma_j^z} \times \prod_{i \in V} e^{-\tau h_i \sigma_i^z}$$

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$$f_{\tau,k}(\theta_{ij,0}, \theta_{ij,1})$$
$$= \langle \psi_{k-1} | e^{-\tau \cdot J_{ij} \cdot Z_i Z_j} \cdot e^{-i(\alpha_{ij} \cdot Z_i Y_j + \beta_{ij} \cdot Y_i Z_j)/2} | \psi_{k-1} \rangle,$$

$$\alpha_{ij}^*, \beta_{ij}^* = \text{arg max } f_{\tau,k}(\alpha_{ij}, \beta_{ij}) \,.$$

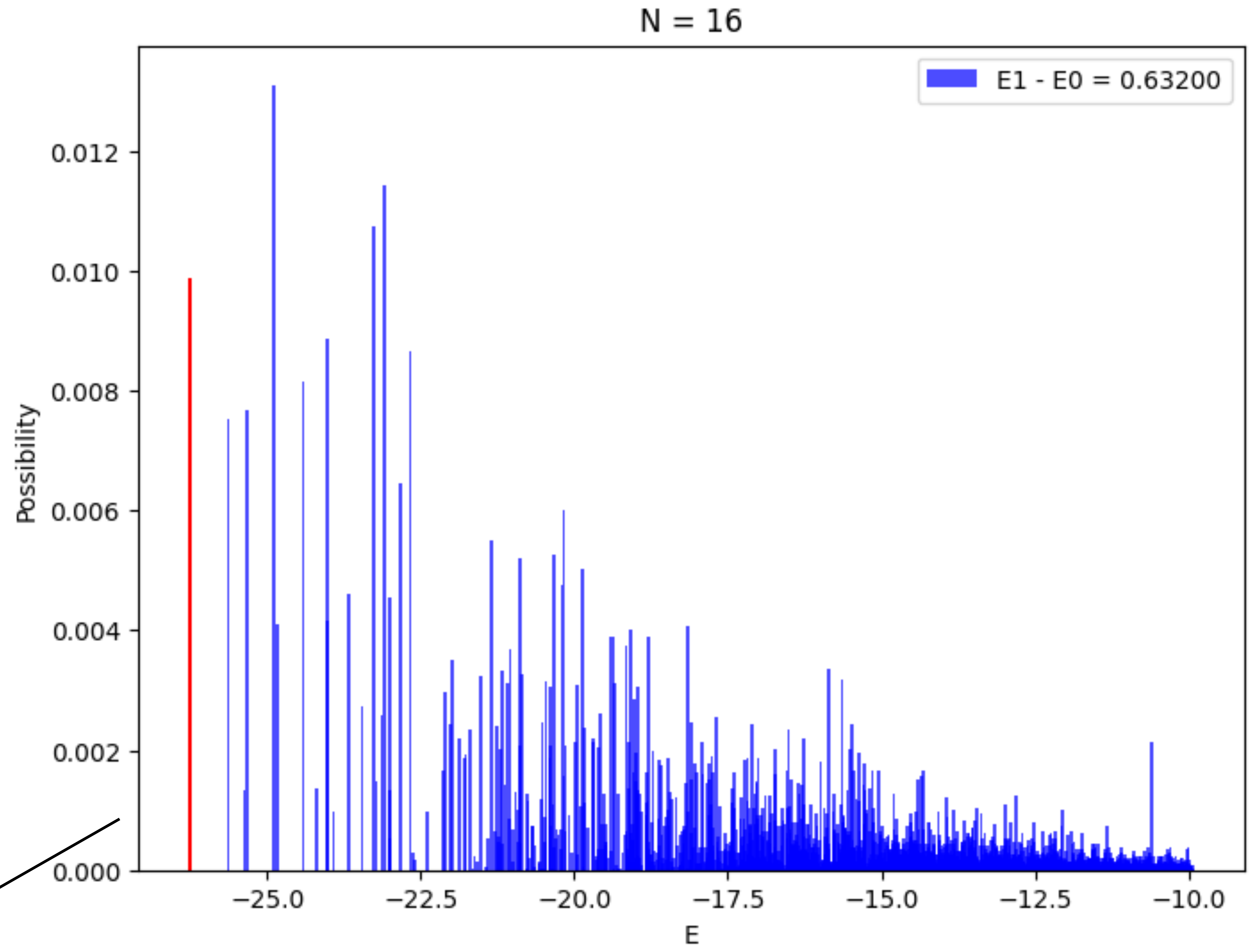
Imaginary time evolution (ITE) of QUBO

$$|\psi_1\rangle = \prod_i R_y(\theta_i)\,|+\rangle^{\otimes N}$$

$$|\psi_2\rangle = e^{-i(\alpha^*_{01} Z_0 Y_1 + \beta^*_{01} Y_0 Z_1)/2}\,|\psi_1\rangle$$

$$|\psi_3\rangle = e^{-i(\alpha^*_{23} Z_2 Y_3 + \beta^*_{23} Y_2 Z_3)/2}\,|\psi_2\rangle$$

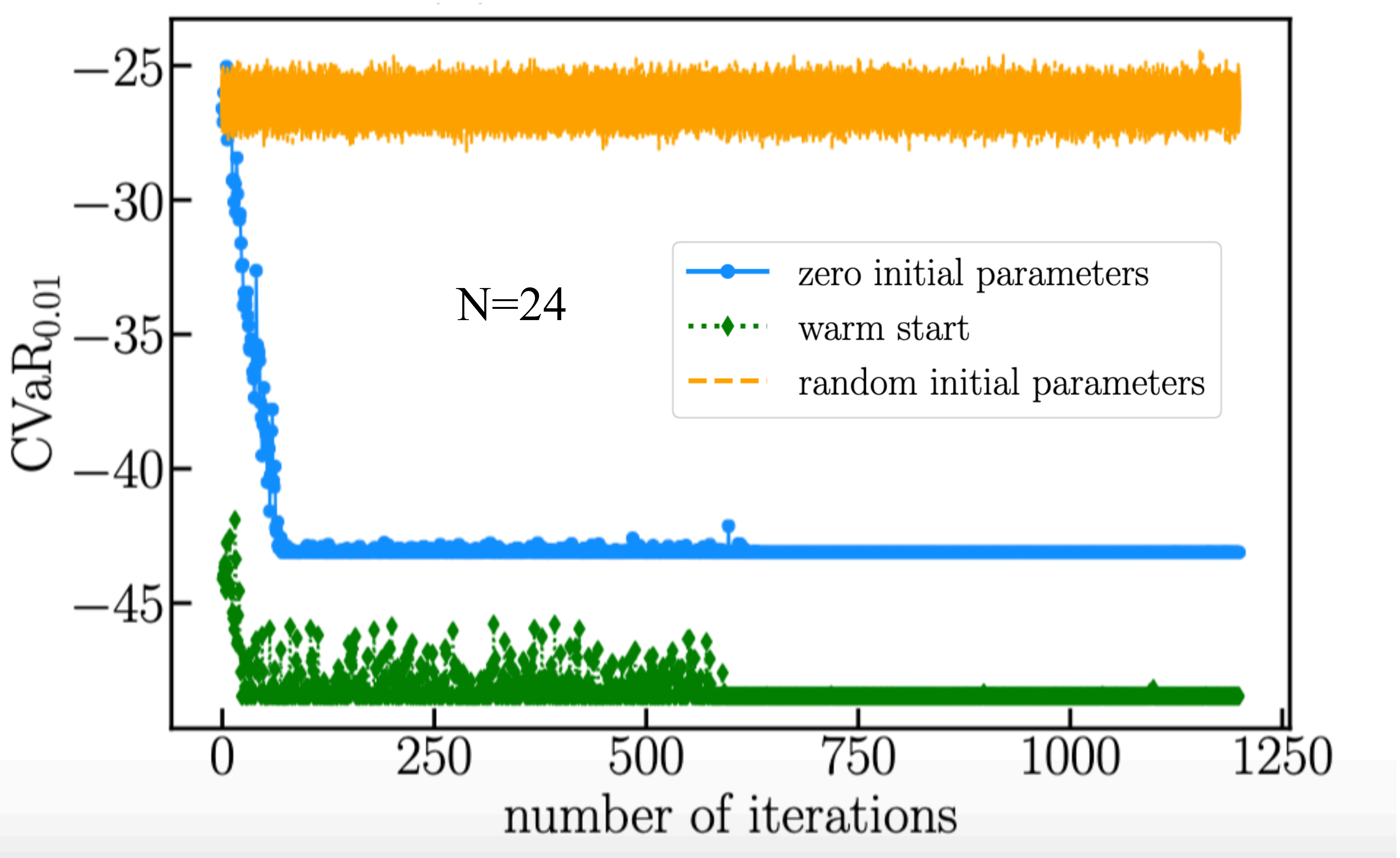
$$\vdots$$



Warm start of VQE

Results

- VQE of different initial parameters for the same instance

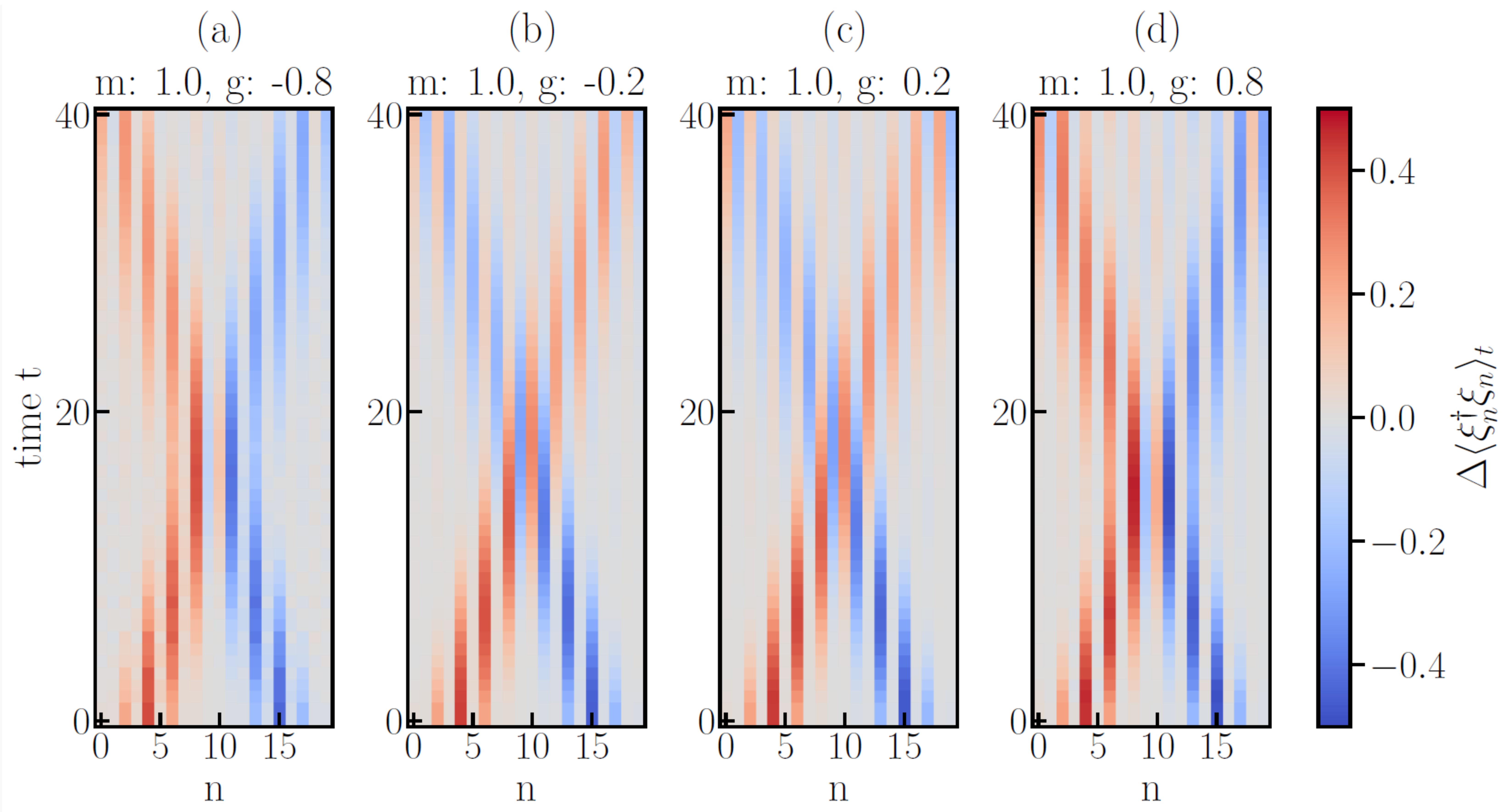


Y. Chai, K. Jansen, S. Kühn, T. Schwägerl, and T. Stollenwerk,
Structure-Inspired Ansatz and Warm Start of Variational Quantum Algorithms for Quadratic Unconstrained Binary Optimization Problems, arXiv:2407.02569.

Real-time dynamics

- Monte Carlo: sign problem
- Tensor network: increasing entanglement

Fermion scattering in Thirring model:



- Elastic scattering between the fermion and antifermion for strong interaction

Y. Chai, A. Crippa, K. Jansen, S. Kühn, V. R. Pascuzzi, F. Tacchino, and I. Tavernelli,
Fermionic Wave Packet Scattering: A Quantum Computing Approach, arXiv:2312.02272. (Accepted by Quantum)

Meson's PDFs in Schwinger model:

$$f(x) = \int_{-\infty}^{\infty} \frac{dz^-}{4\pi} e^{-ixz^- P^+} \langle h(P)| \bar{\psi}(z^-)\gamma^+\psi(0) |h(P)\rangle$$

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$$f(x) = \frac{a}{4\pi N} \sum_{mn} e^{ixM(n-m)a} \langle h| e^{-iH(n-m)a}\psi^\dagger(0, na)e^{iH(n-m)a}(I + \gamma^0\gamma^1)\psi(0, ma) |h\rangle$$

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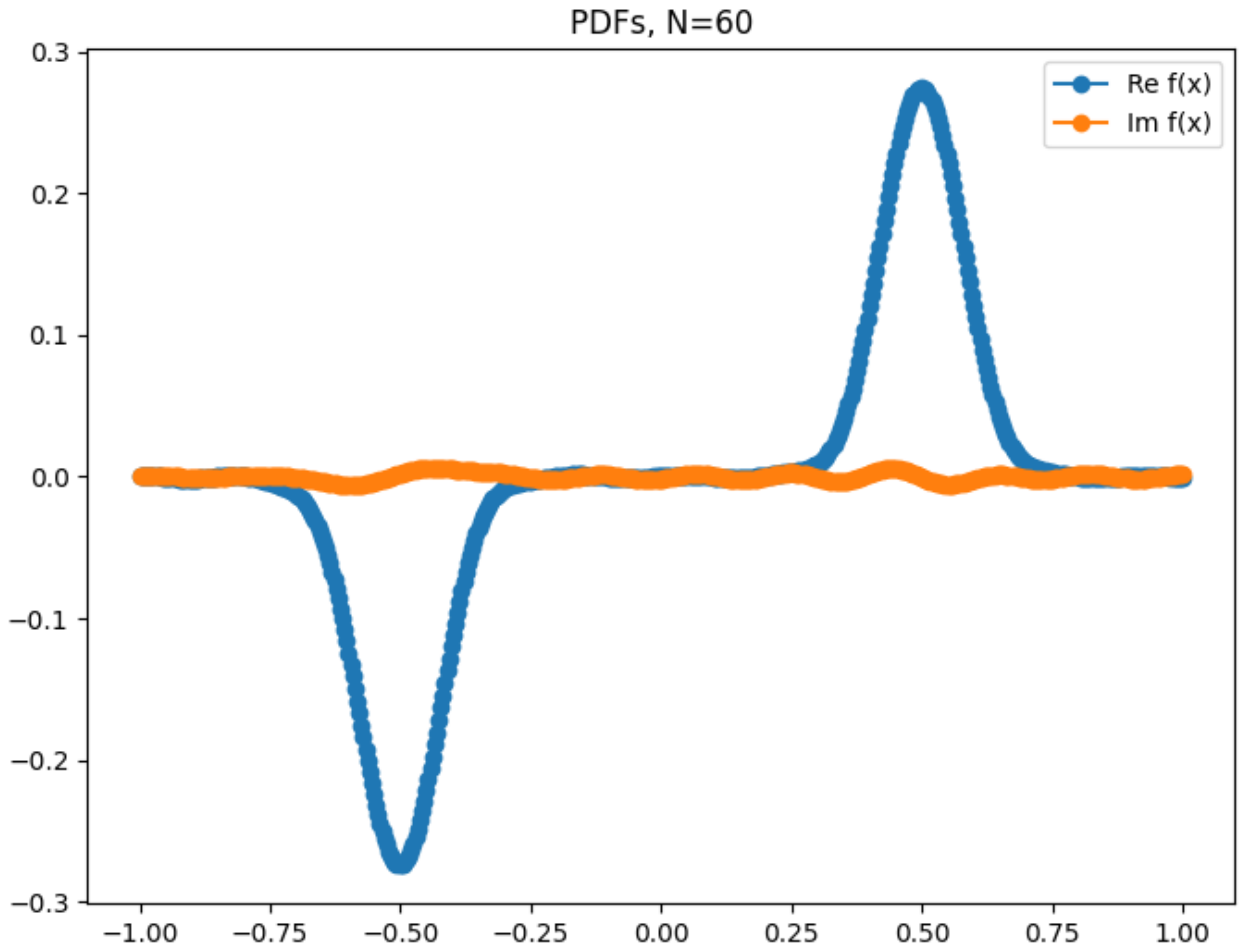


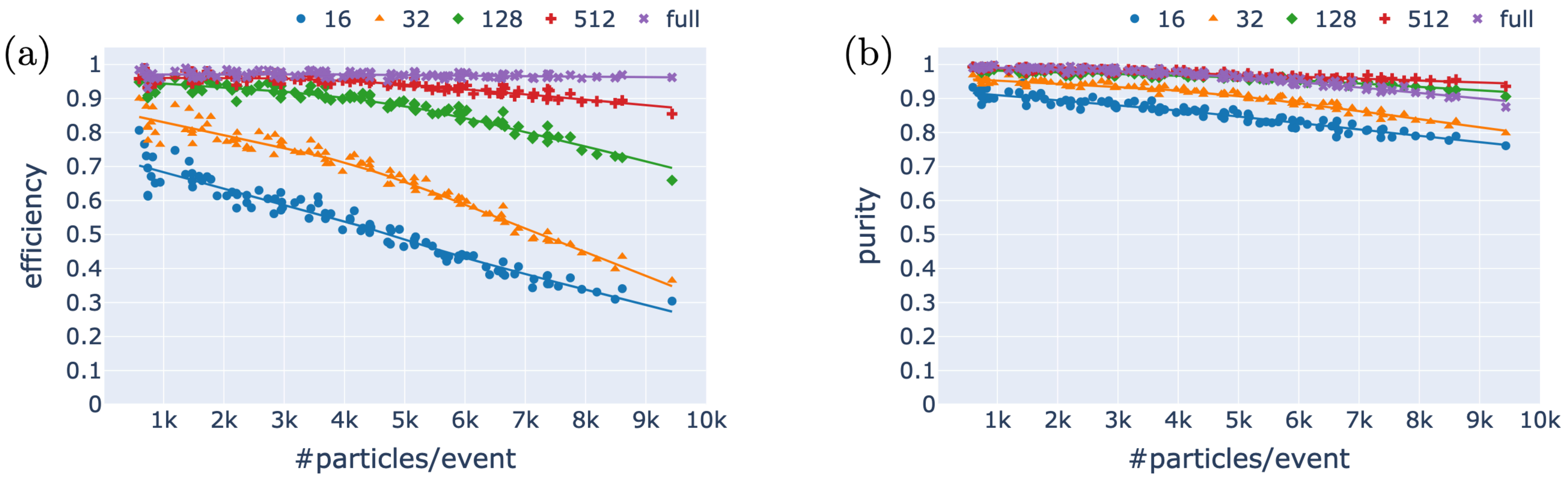
Summary and outlook:

- Quantum optimization in HEP
    - Particle tracking — Variational Quantum Eigensolver (VQE)
    - Structure-inspired ansatz and warm start of VQE
    - Other applications of VQE and warm start approach in HEP experiment?
    - Larger system size?

- Short introduce of real-time dynamics of HEP in quantum computing
    - Particle scattering in a fermonic model
        - Meson scattering
        - Related with the experiments?
    - Meson's Parton distribution functions (PDFs) in Schwinger model
        - Multi-flavor?
        - Higher dimensions?

Appendix

Divide problems to sub-QUBO



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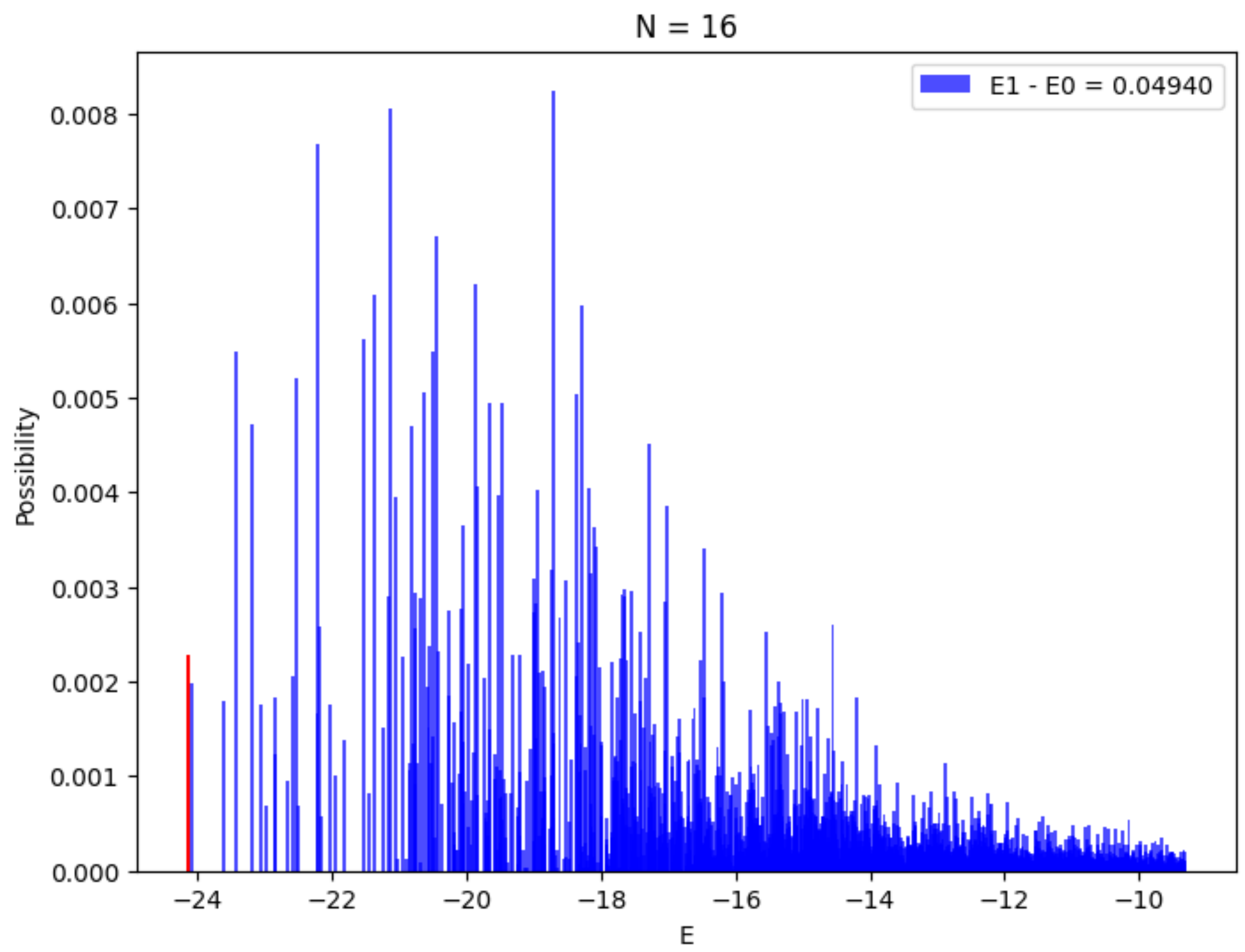
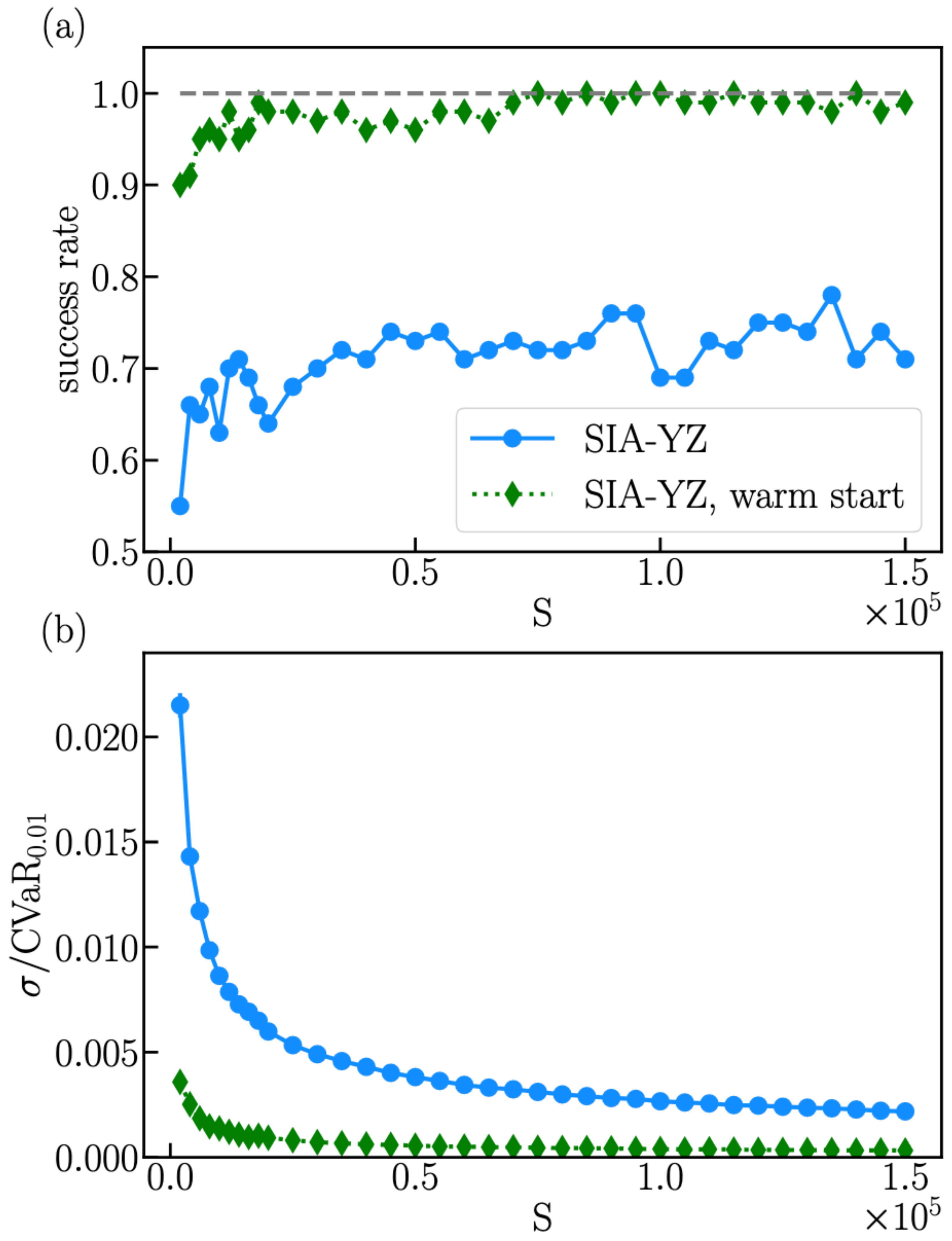
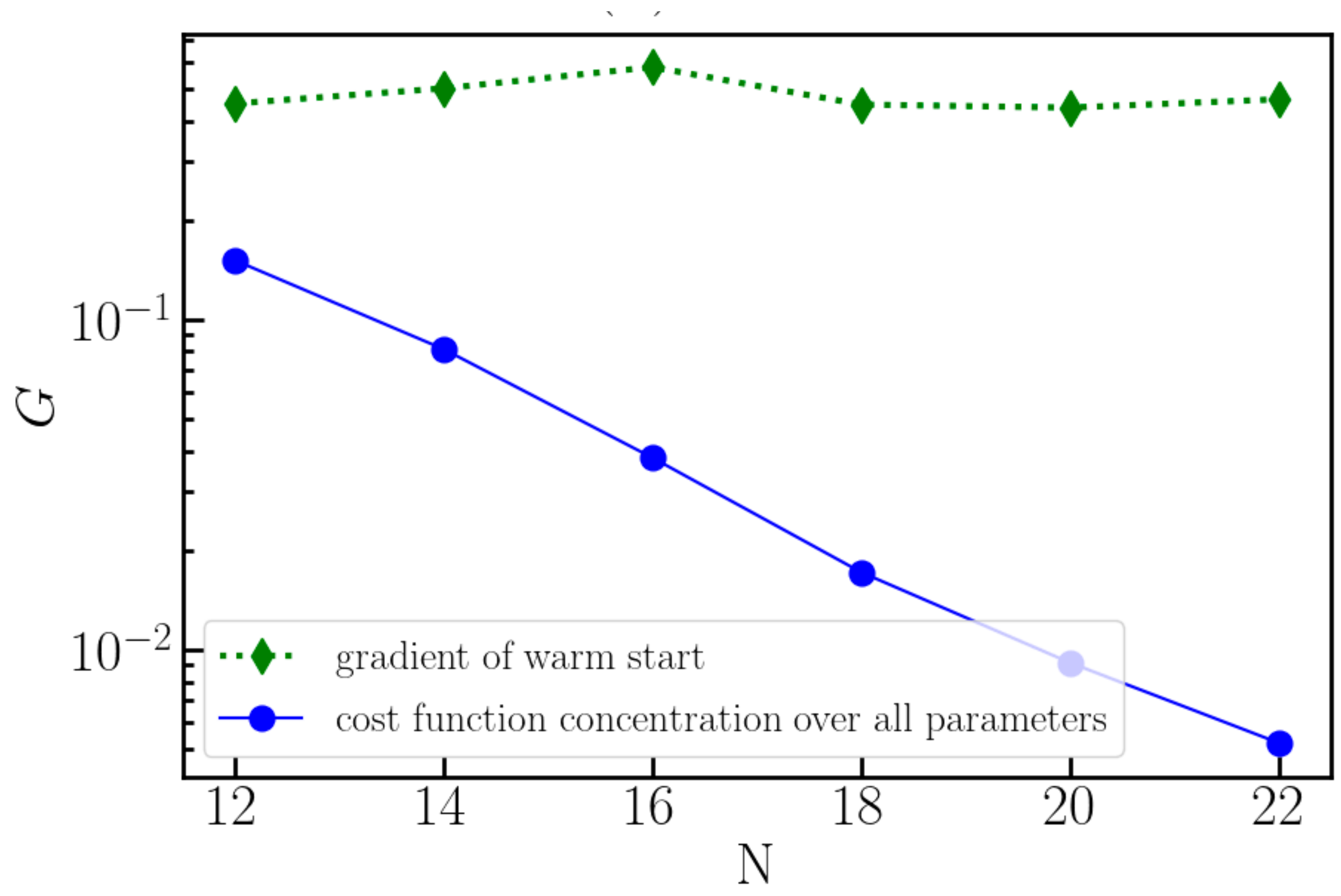


Results

- Statistic error



- Barren plateau



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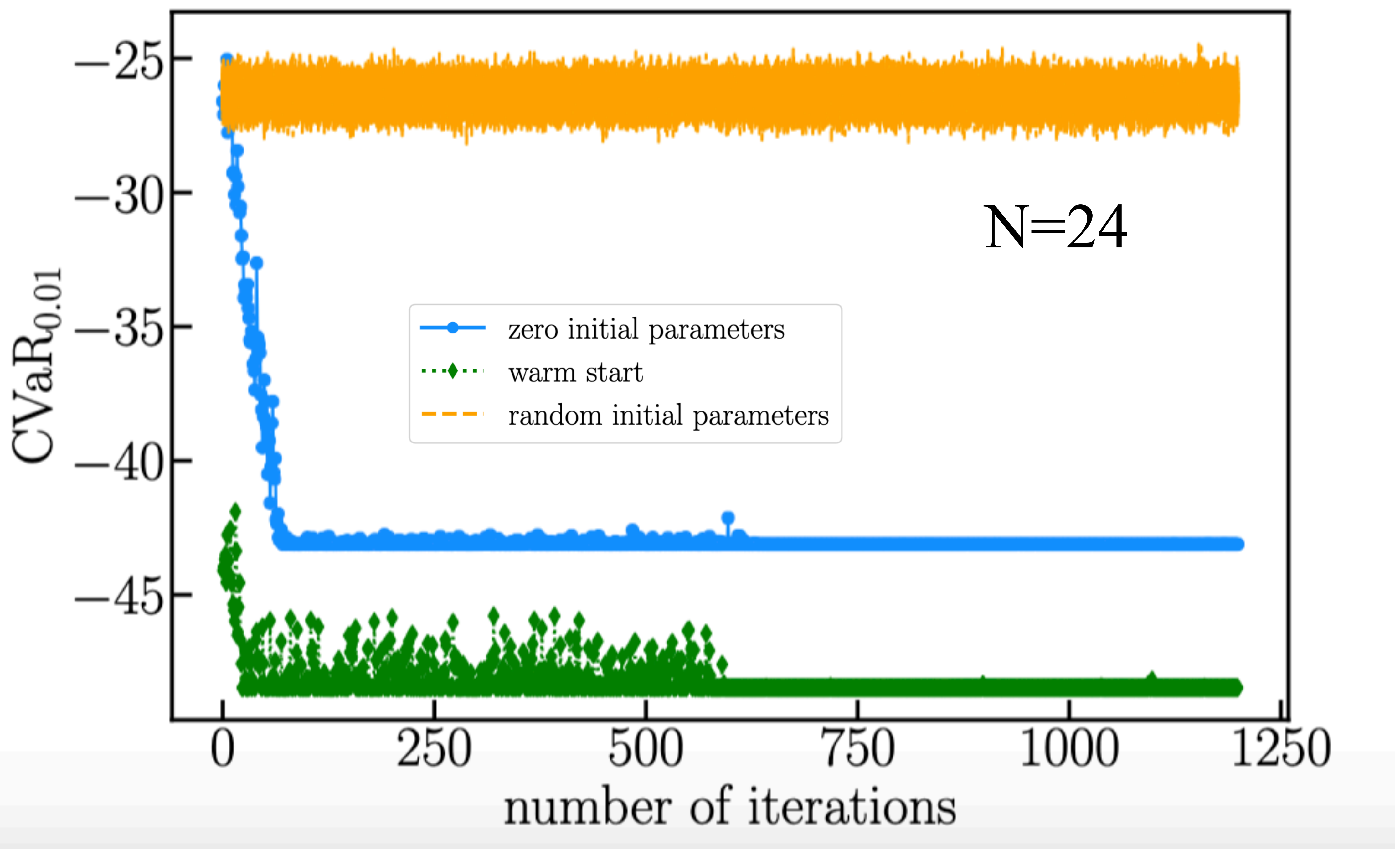

- Success rate of finding the ground state