Optimizing QUBO on Digital Quantum Computers: From Particle Tracking to Scalable Algorithms

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In collaboration with Alice Di Tucci

DESY. QUANTUM | Center for Quantum Technology and Applications

Outline

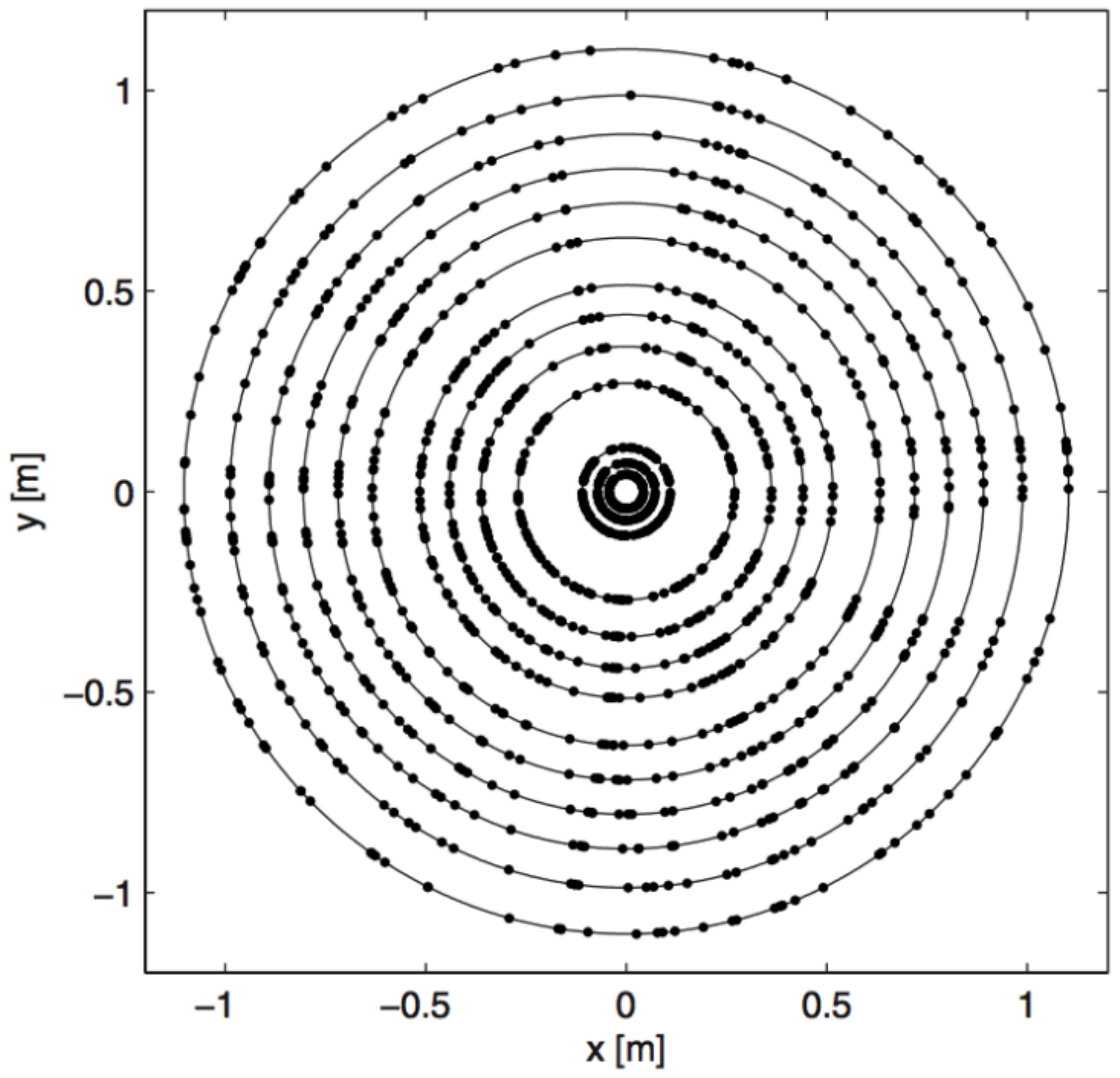
- Particle tracking to **Q**uadratic **U**nconstrained **B**inary **O**ptimization (QUBO) problem

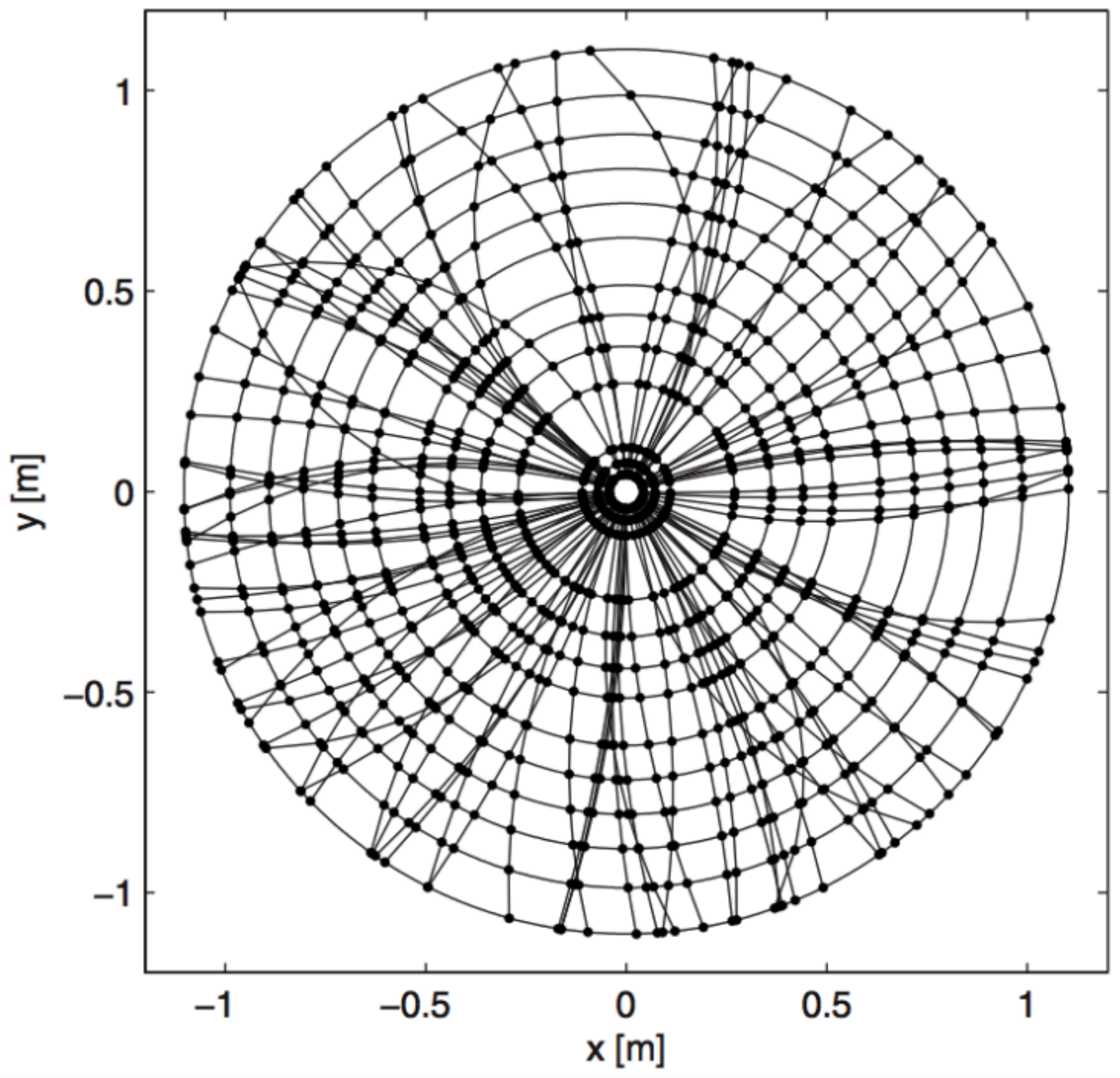
- Quantum algorithms for QUBO problem
  - Variational quantum algorithm, VQE, QAOA….
  - Imaginary Time Evolution-Mimicking Circuit (ITEMC)
    - Fewer measurements, shallower circuits
    - Experiments of 40, 60, 80 qubits on IBM quantum device

- Summary and outlook

Particle tracking

Zlokapa A, Anand A, Vlimant J-R, Duarte JM, Job J, Lidar D, Spiropulu M.
Charged particle tracking with quantum annealing-inspired optimization. Quantum Mach Intell 3, 2021





- Denby-Peterson method

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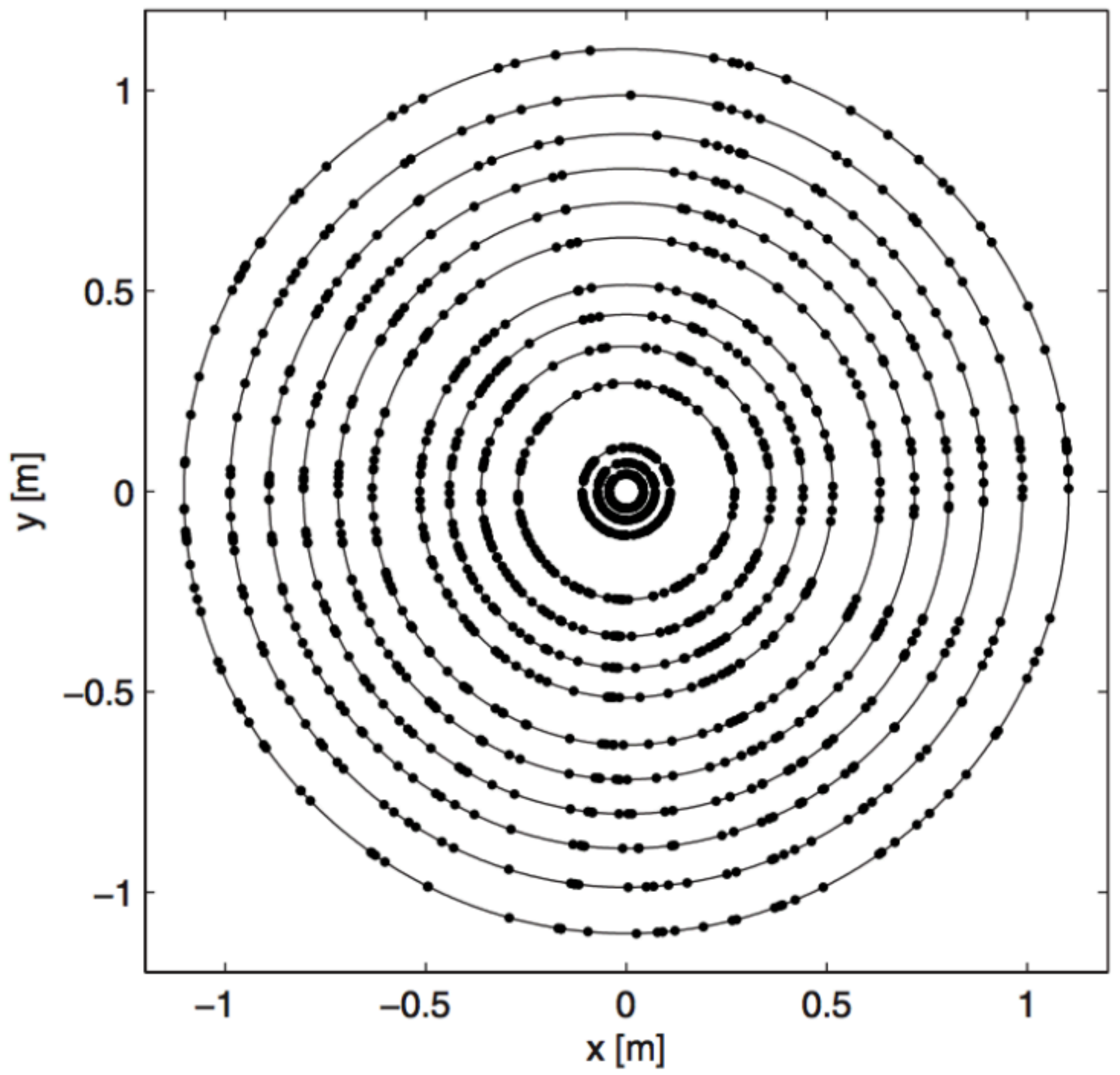
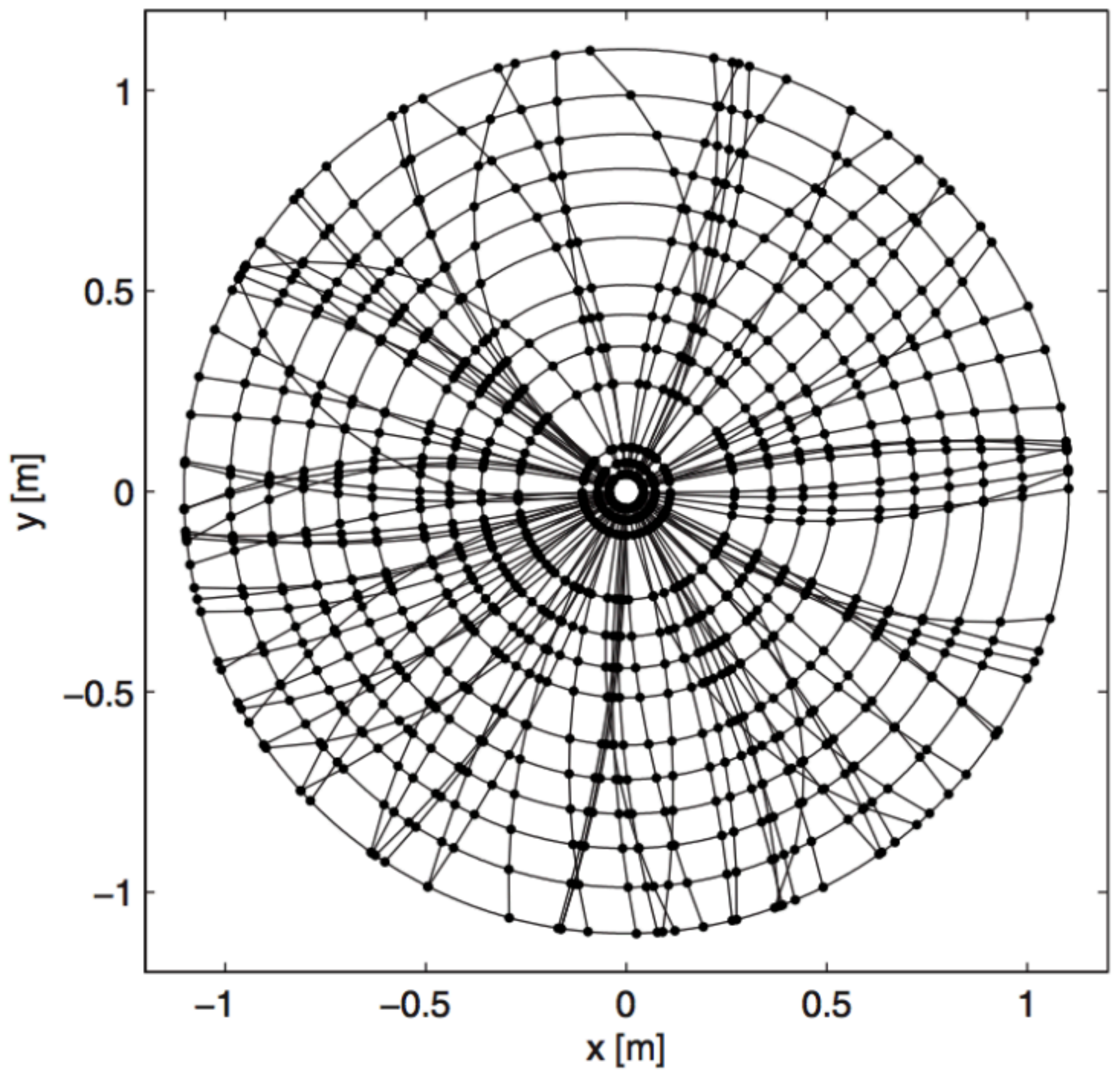
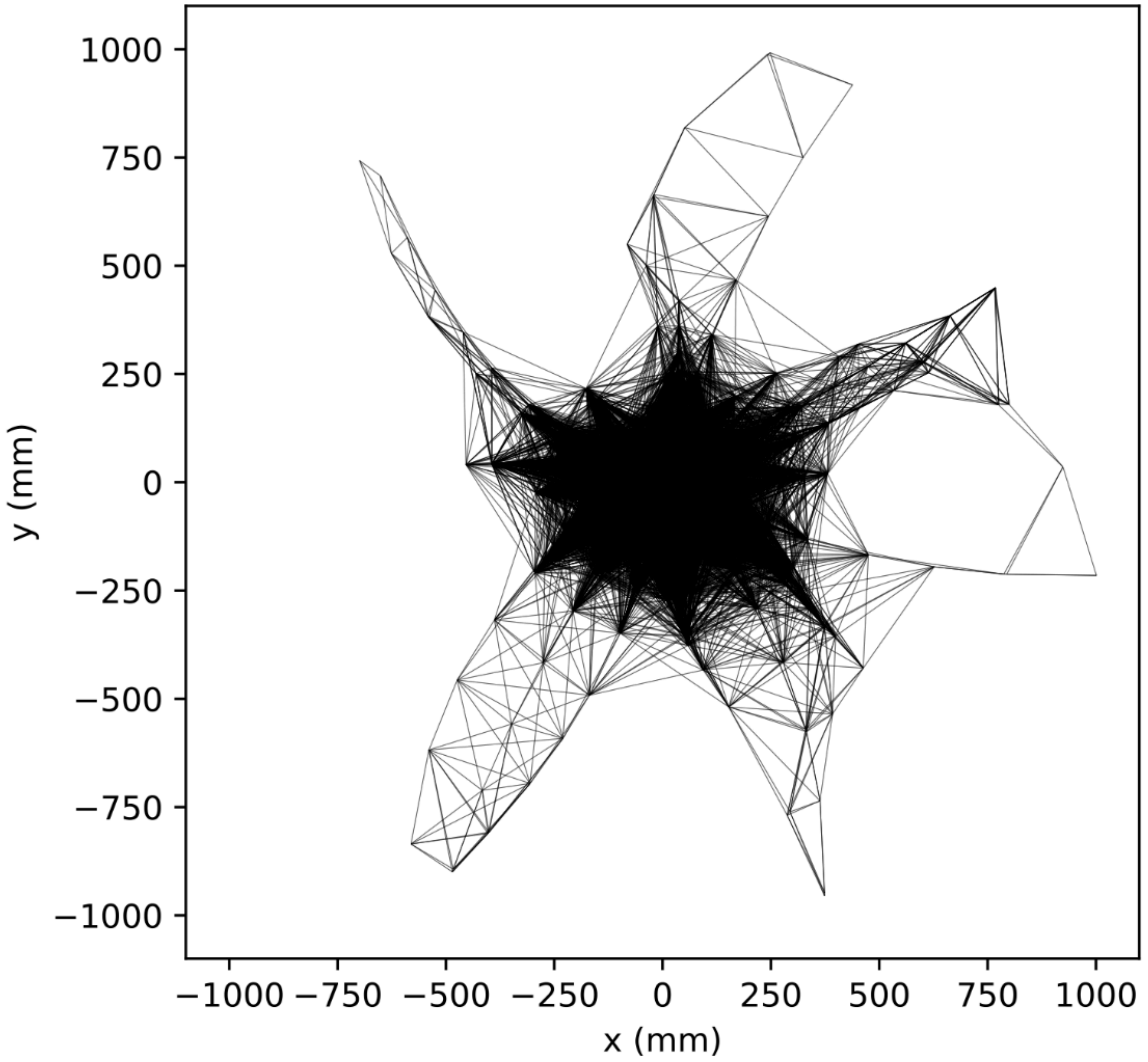




- Denby-Peterson method

All pre-selected potential edges



s_{ab}: edge between hits a and b

s_{ab}= 1: correct edge

s_{ab}= 0: incorrect edge

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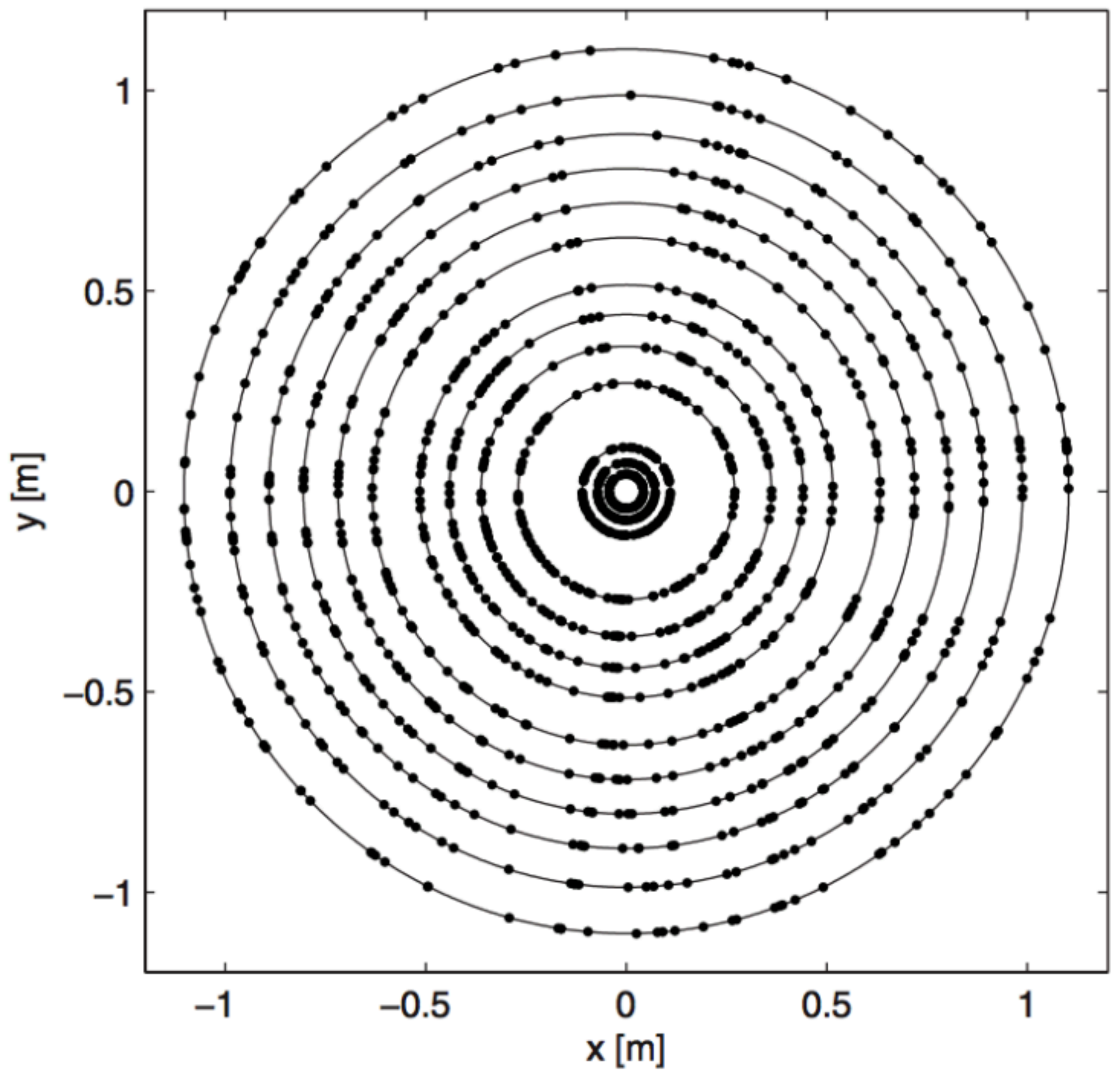
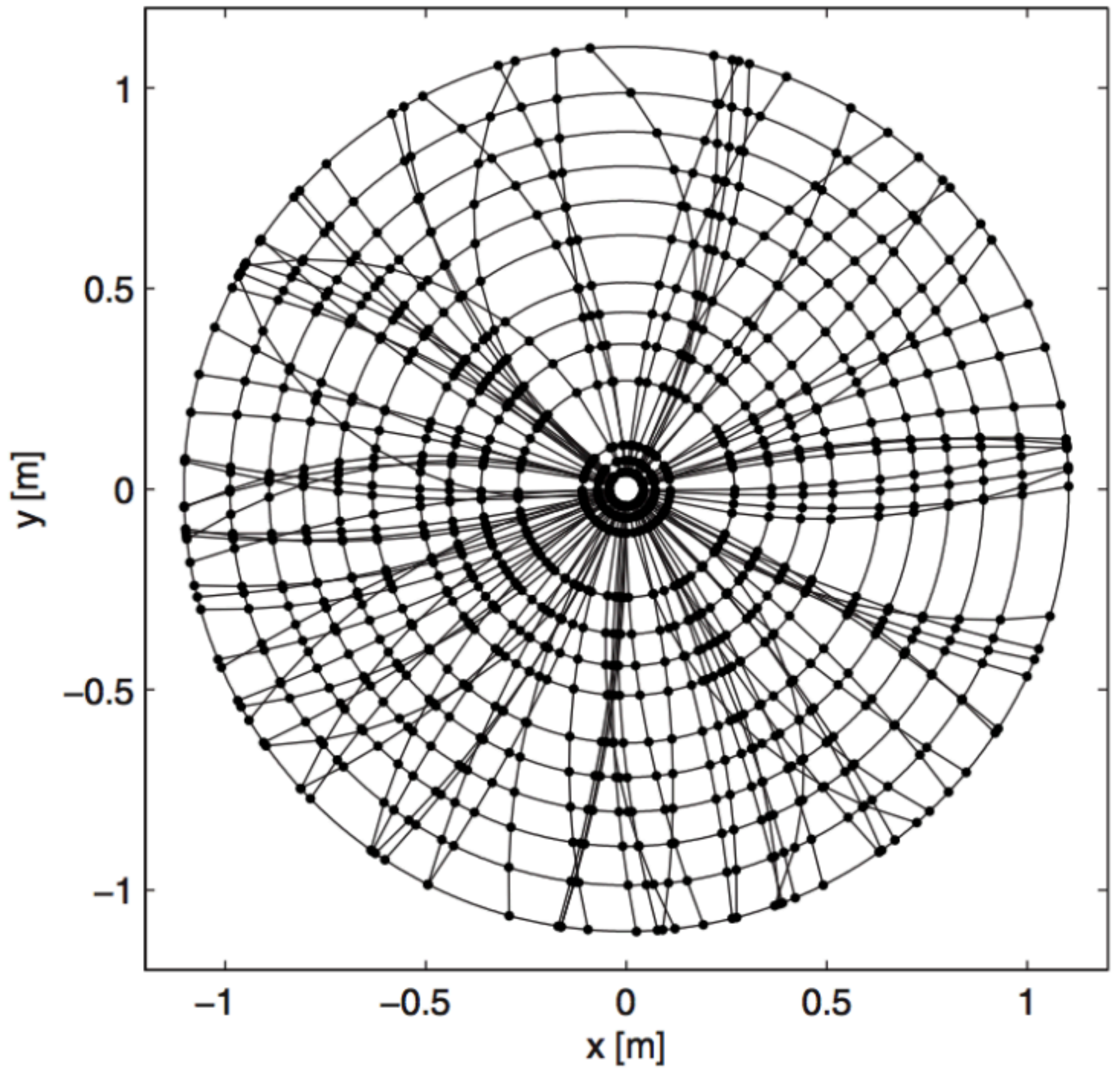
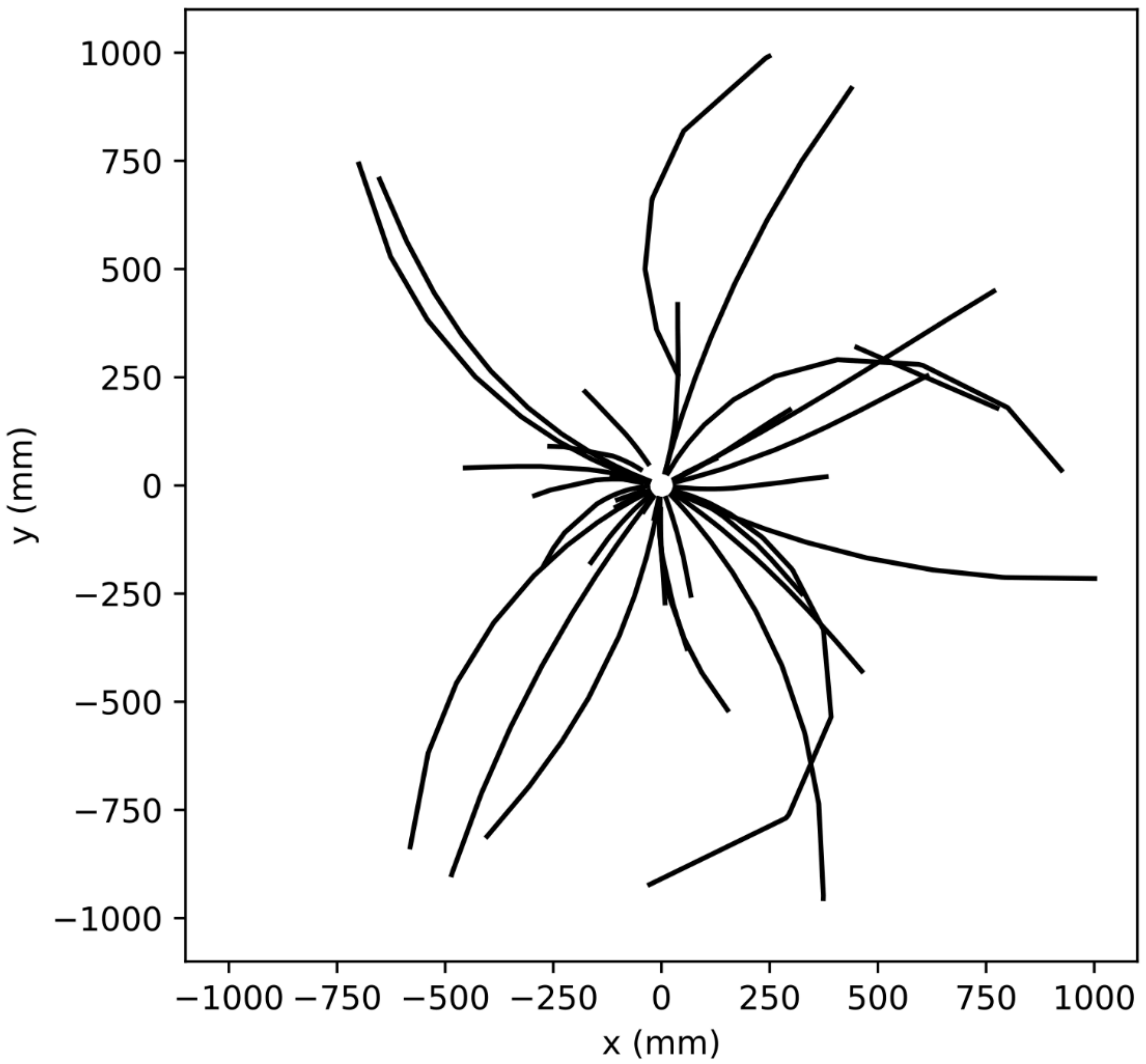




- Denby-Peterson method

After optimization



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- Cost function

$$E = -\frac{1}{2}\left[\sum_{a,b,c}\left(\frac{\cos^{\lambda}\theta_{abc}}{r_{ab}+r_{bc}}s_{ab}s_{bc}\right) - \alpha\left(\sum_{b\neq c}s_{ab}s_{ac} + \sum_{a\neq c}s_{ab}s_{cb}\right) - \beta\left(\sum_{a,b}s_{ab} - N\right)^2\right]$$

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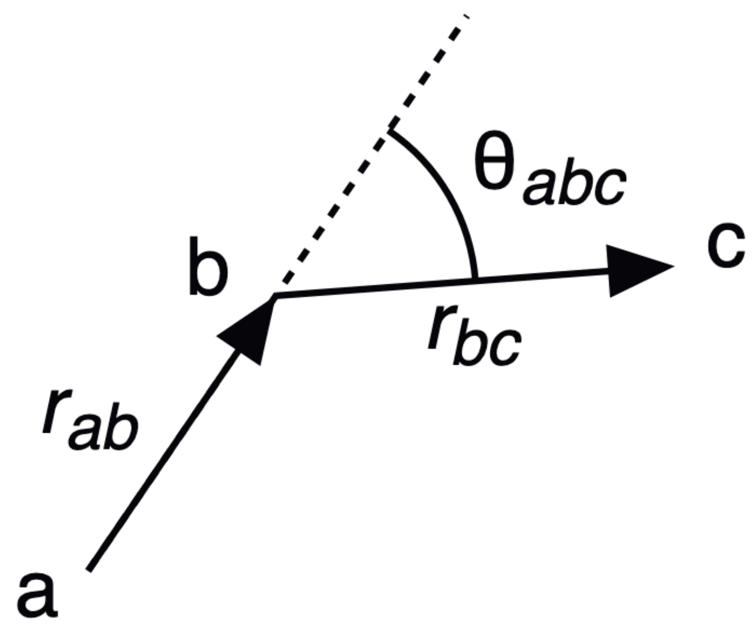
Main term



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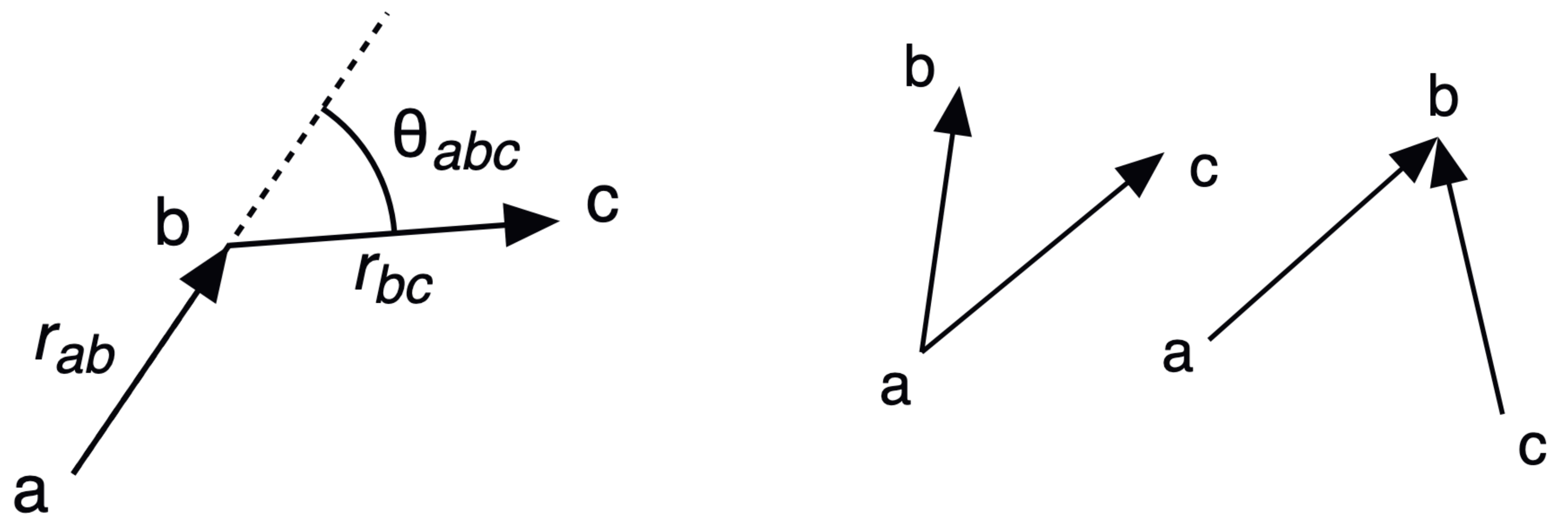
Main term

Penalty term



Edge number = hits number

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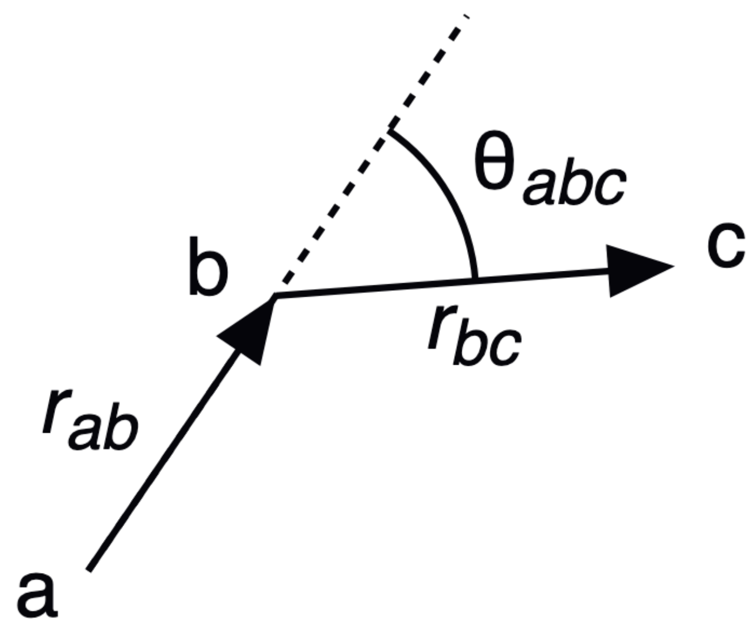

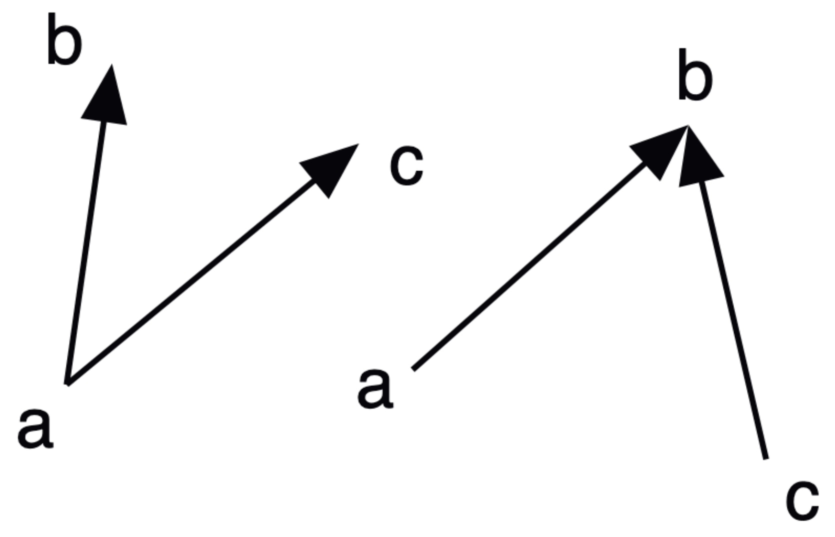

Edge number = hits number

Quadratic **U**nconstrained **B**inary **O**ptimization (QUBO) problem

Particle tracking

- Minimize cost function $s_{ab} \rightarrow s_i$

$$E = \sum_i h_i s_i + \sum_{ij} J_{ij} s_i s_j$$

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$s_i \rightarrow (I - Z_i)/2$

- Find the ground state of a Hamiltonian

$$H = \sum_i h_i \frac{I - Z_i}{2} + \sum_{ij} J_{ij} \left(\frac{I - Z_i}{2}\right)\left(\frac{I - Z_j}{2}\right)$$

Particle tracking

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$$\left(\frac{I - Z_i}{2}\right)|0\rangle = 0$$

$$\left(\frac{I - Z_i}{2}\right)|1\rangle = |1\rangle$$

$$\left(\frac{I - Z_i}{2}\right)|s_i\rangle = s_i|s_i\rangle$$

$$H|s_0 s_1 \cdots\rangle = E|s_0 s_1 \cdots\rangle$$

Particle tracking

- Minimize cost function $s_{ab} \rightarrow s_i$

$$E = \sum_i h_i s_i + \sum_{ij} J_{ij} s_i s_j$$

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

- Find the ground state of a Hamiltonian

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

$$H | s_0 s_1 \cdots \rangle = E | s_0 s_1 \cdots \rangle$$

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Quantum Algorithms

- Get the ground state bit string from measurements

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

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Quantum Algorithms

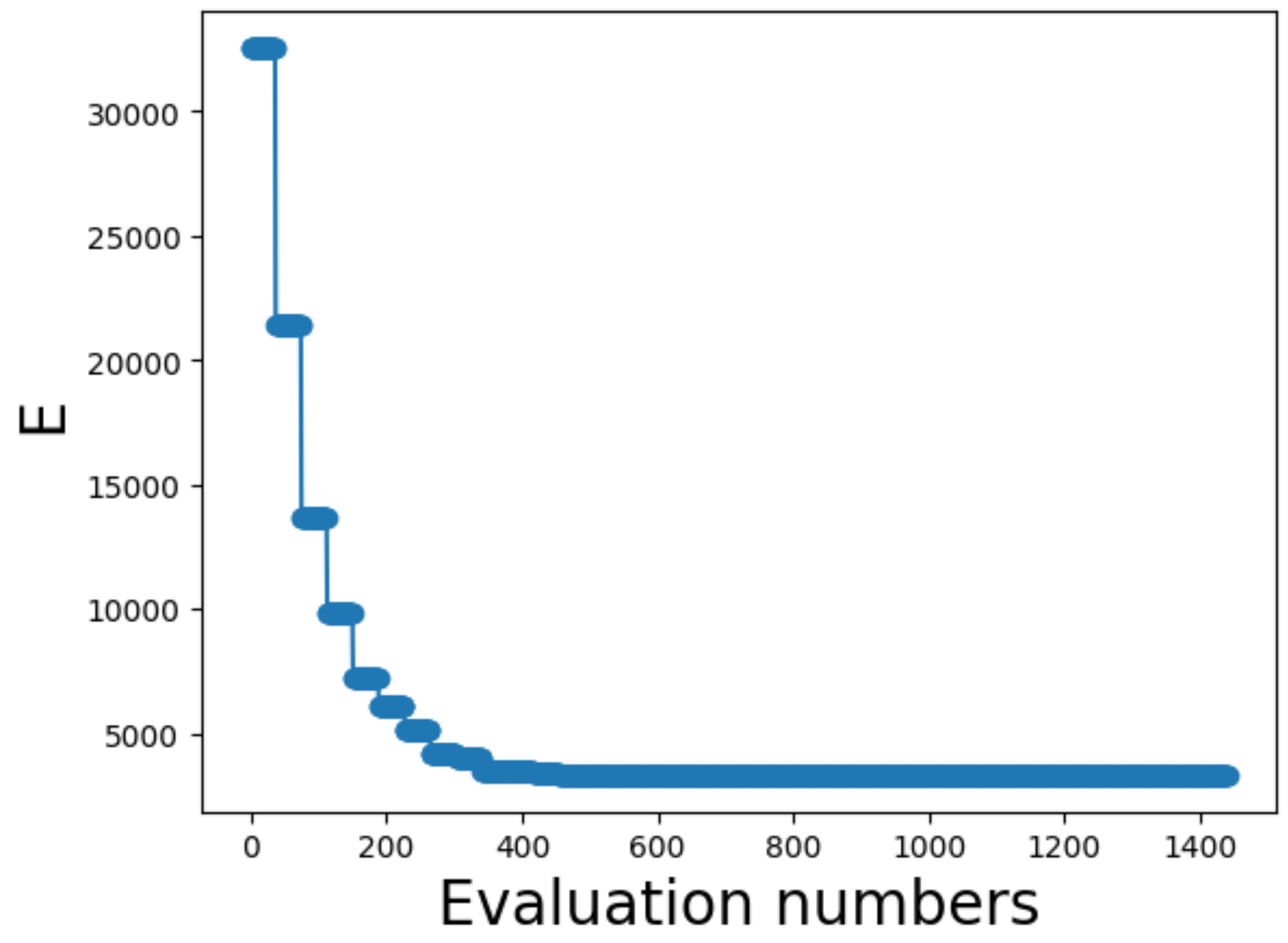
- Get the ground state bit string from measurements

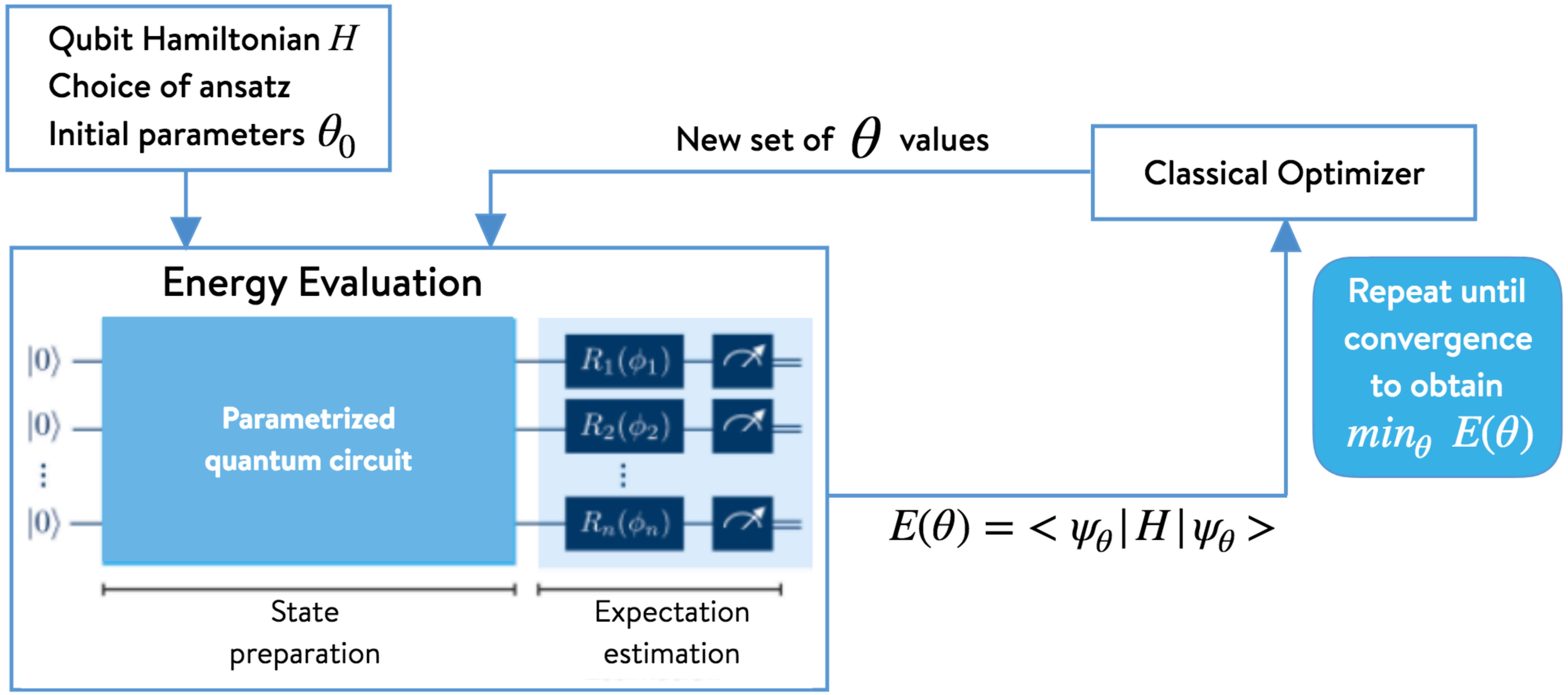
$e.g., |111000\rangle$

- Got the solution

Segments s_0, s_1, s_2 are true

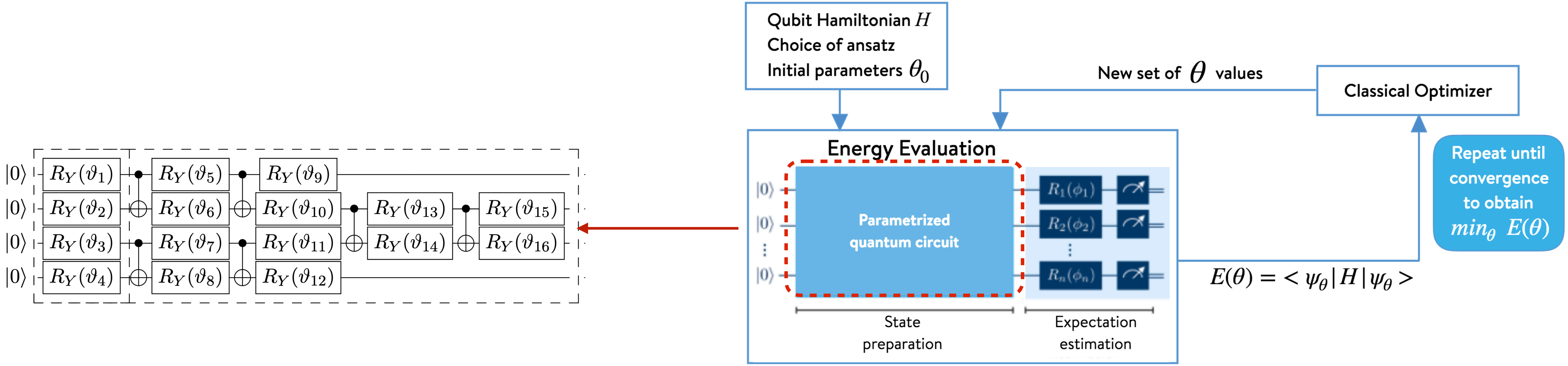
Variational Quantum Algorithm (VQA)





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

Variational Quantum Eigensolver(VQE)



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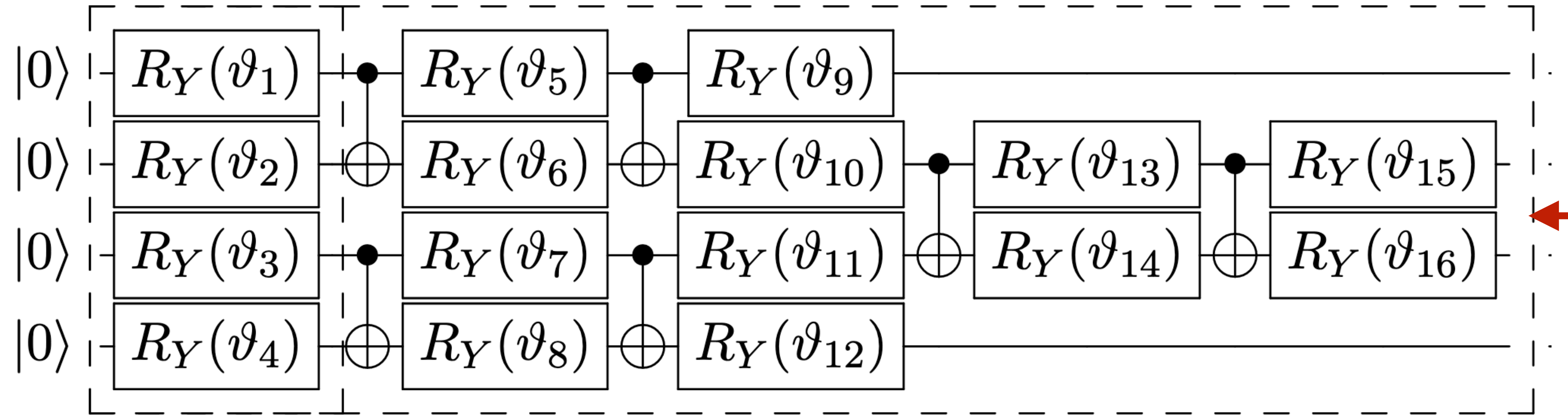

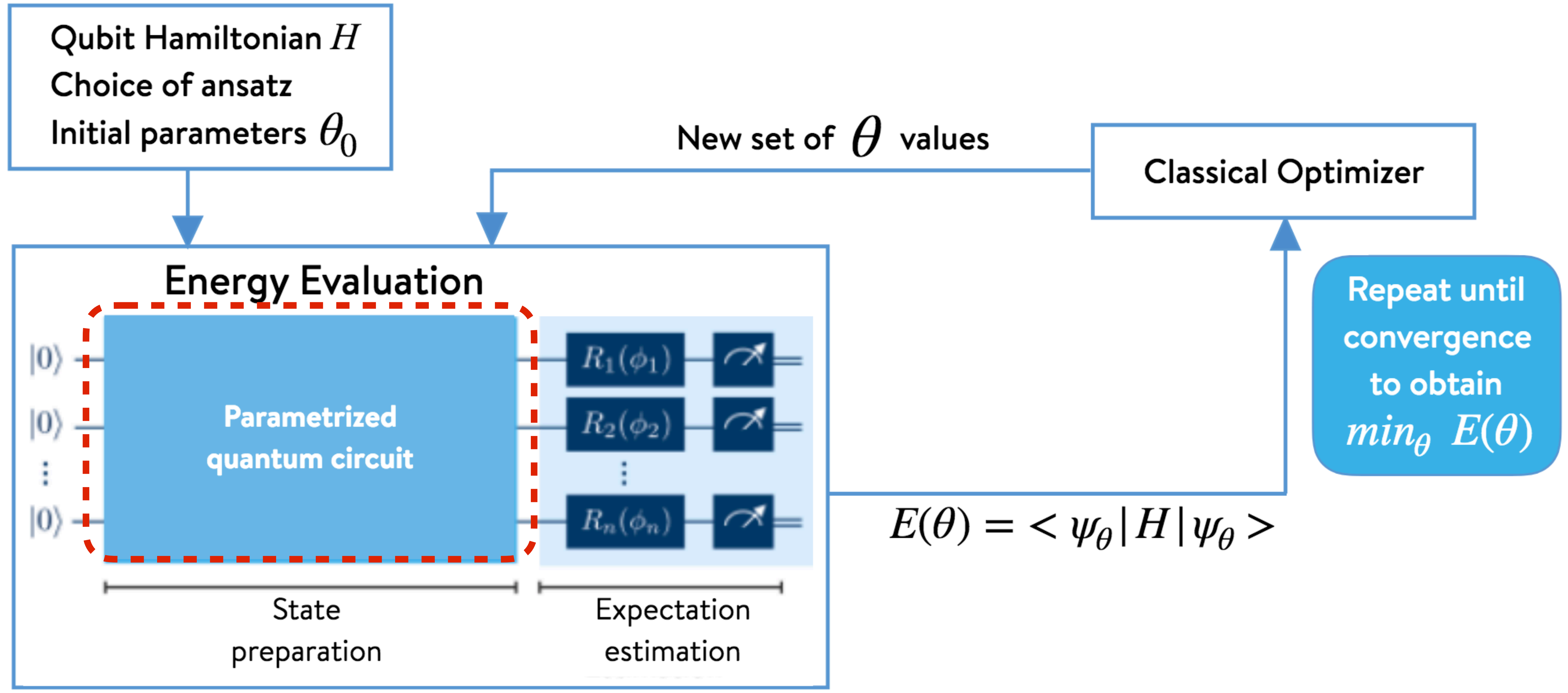

- Good: Flexible, shallow circuit
  - Bad: Parameter initialization, optimization, measurements

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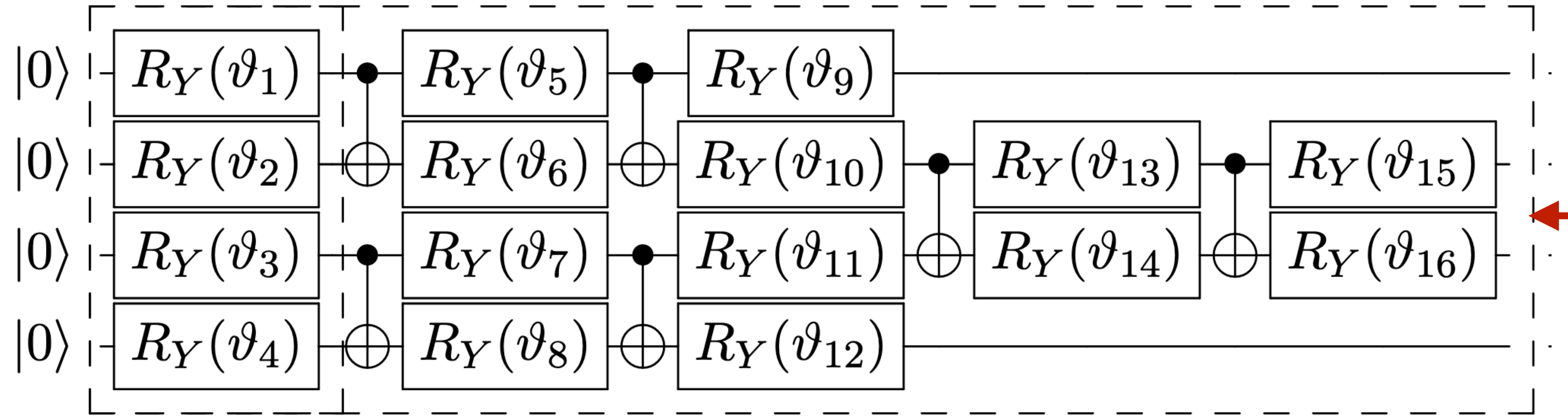

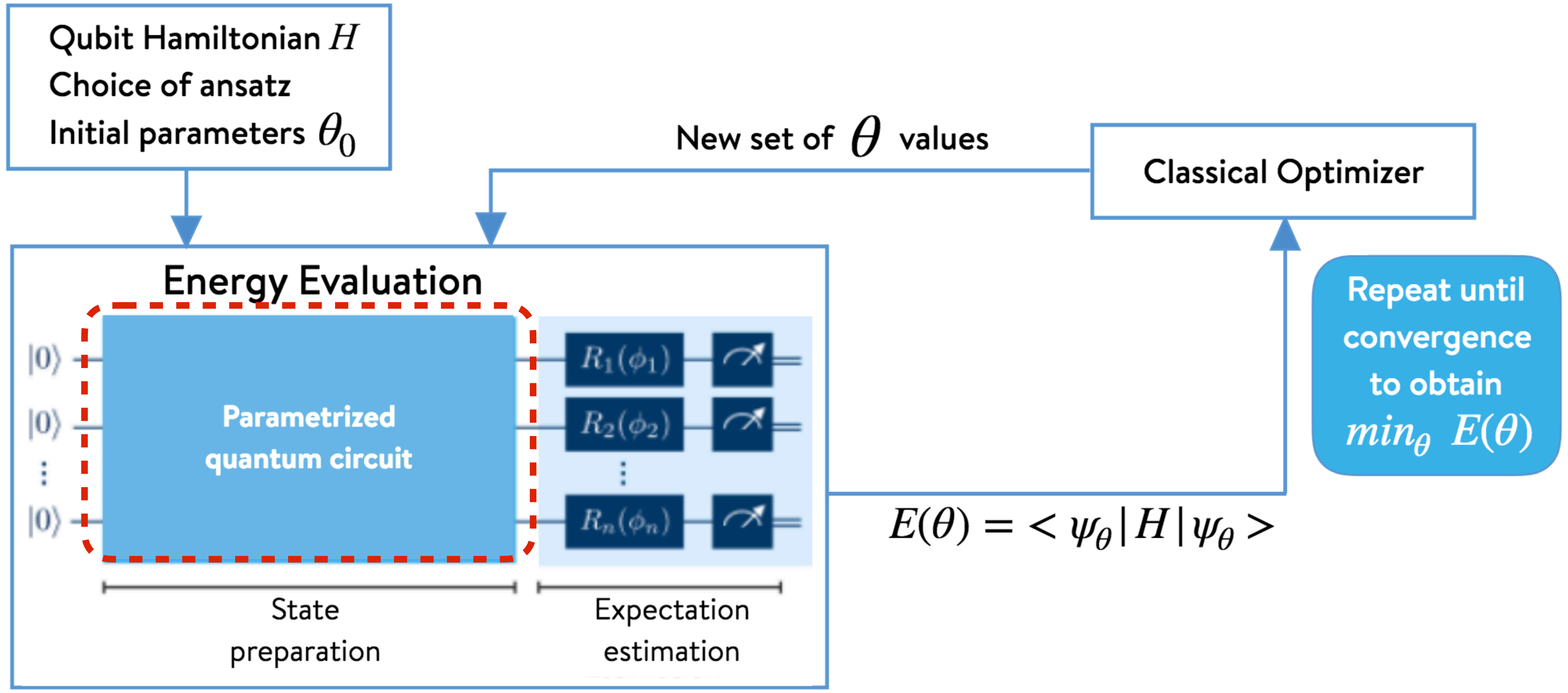

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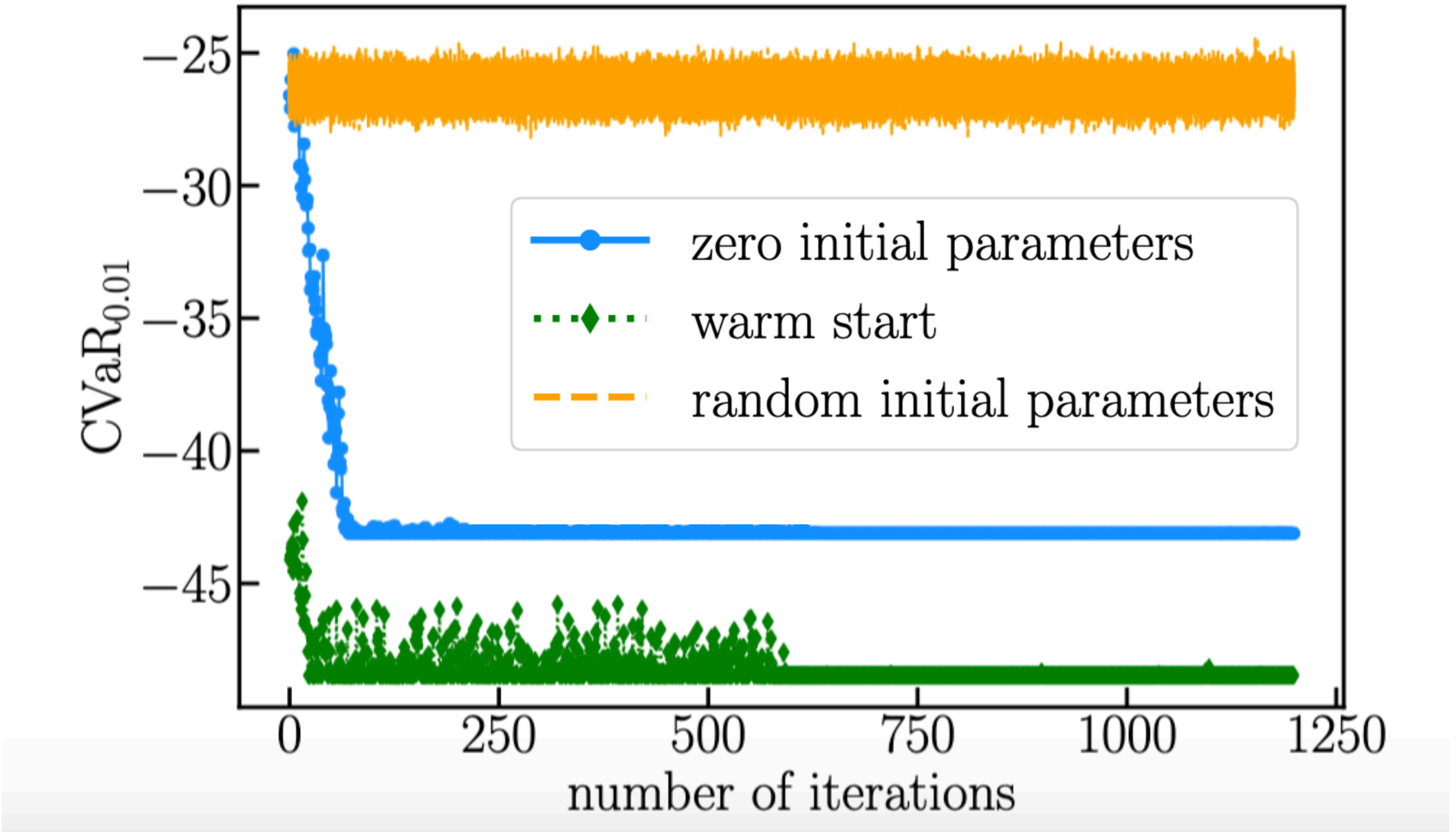
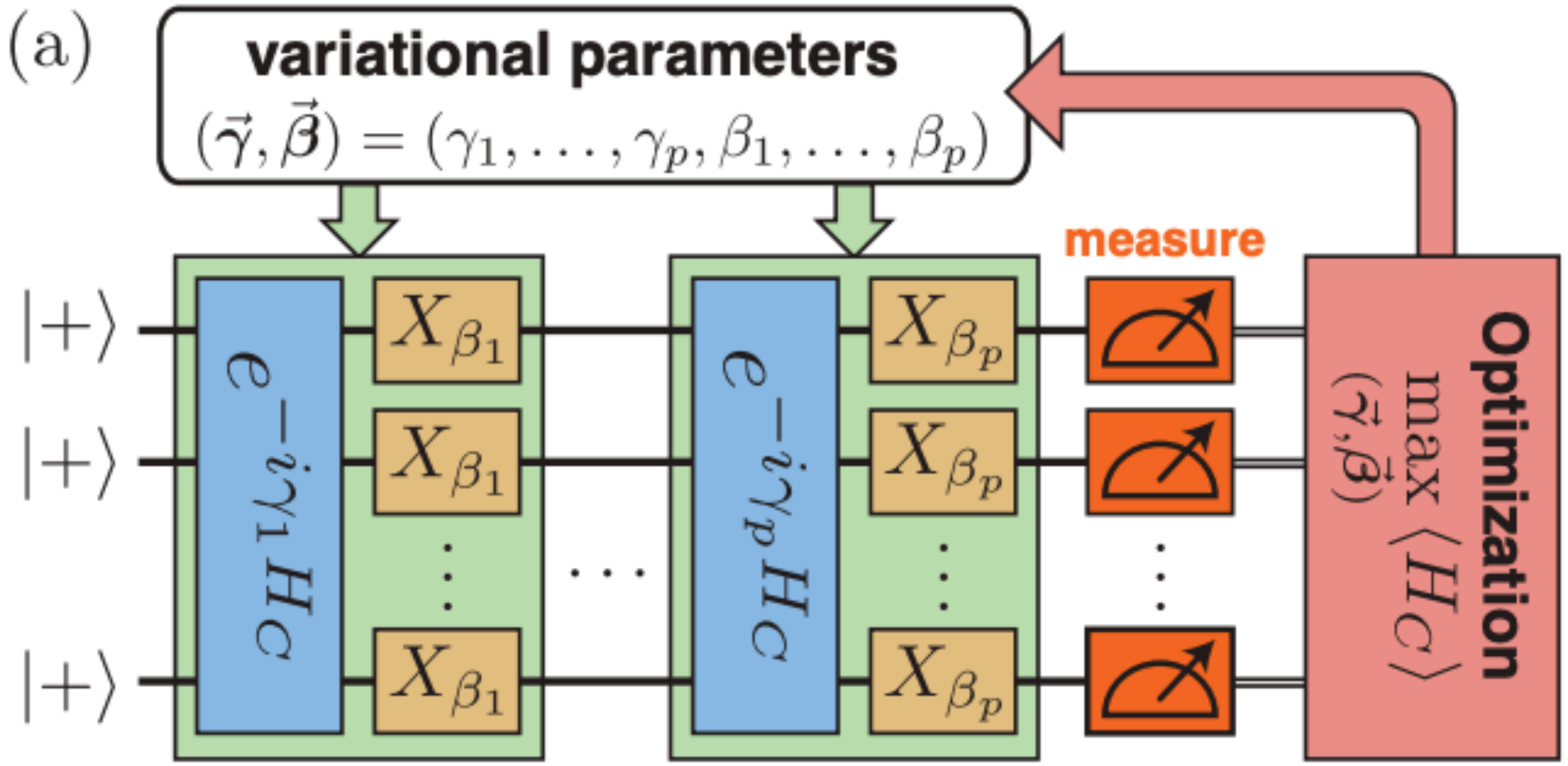


Quantum Approximate Optimization Algorithm (QAOA)



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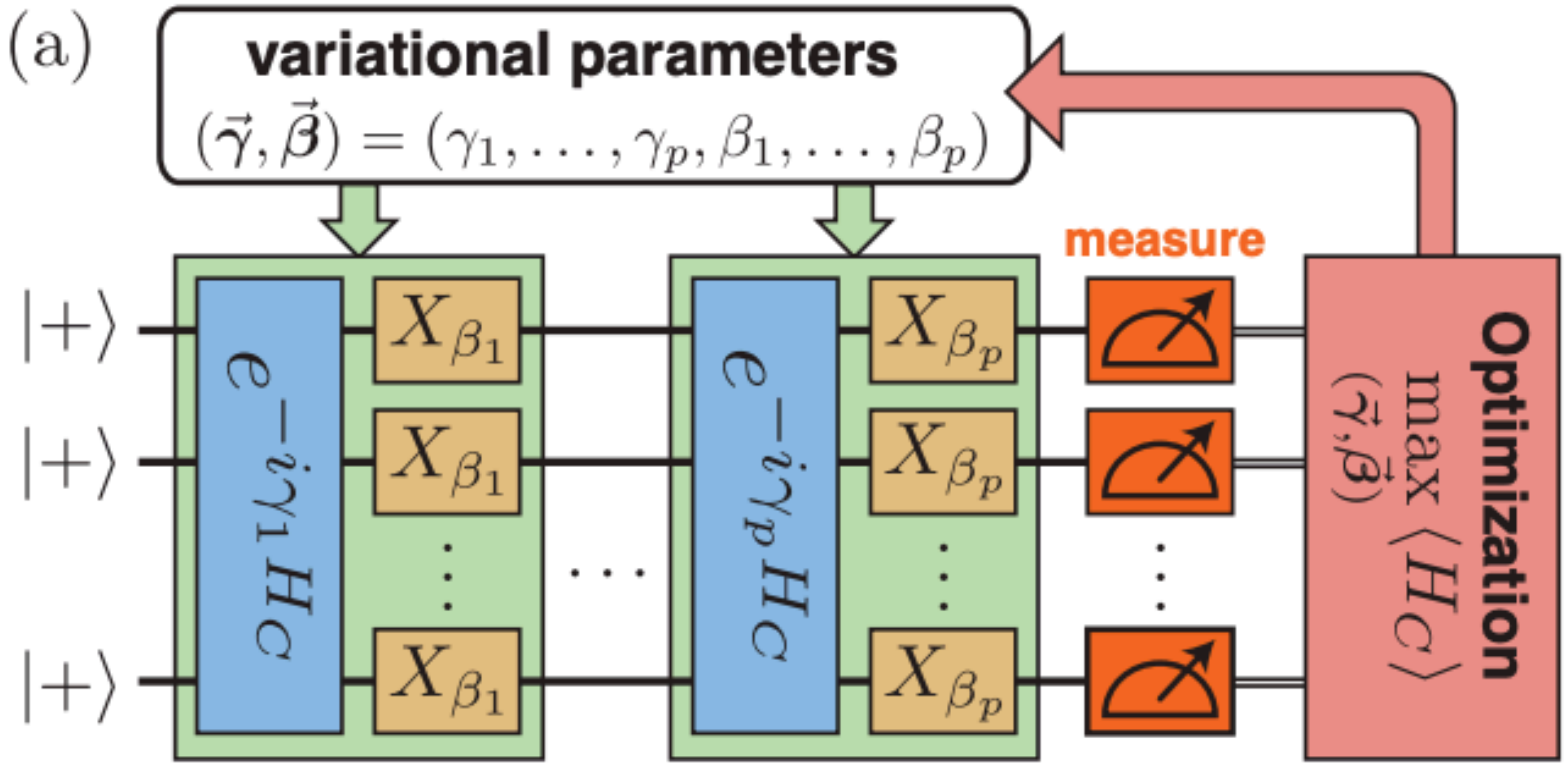

- Good: physical guarantee, less parameters
  - Bad: deep circuit, measurements

Requirements of more practical algorithms…

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- Physical theorem

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- Shallow quantum circuit

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- Fewer measurements

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- Physical theorem

The Imaginary time evolution of the QUBO Hamiltonian:

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

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

$$\to a_0|E_0\rangle + e^{-\tau E_1}a_1|E_1\rangle + \cdots$$

$$\xrightarrow{\tau\to\infty} |E_0\rangle$$

- Shallow quantum circuit

- Fewer measurements

Requirements more practical algorithm…

- Physical theorem

Can we find a quantum circuit to mimic the Imaginary time evolution?

$$U|+\rangle^{\otimes N} \sim e^{-\tau \cdot H} \cdot |+\rangle^{\otimes N}$$

- Shallow quantum circuit

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Requirements more practical algorithm…

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Non-unitary

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Normalization

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Non-unitary

Normalization

- $\tau \to \infty$, large correlation, deep circuit
- τ small, short circuit depth, but low success rate

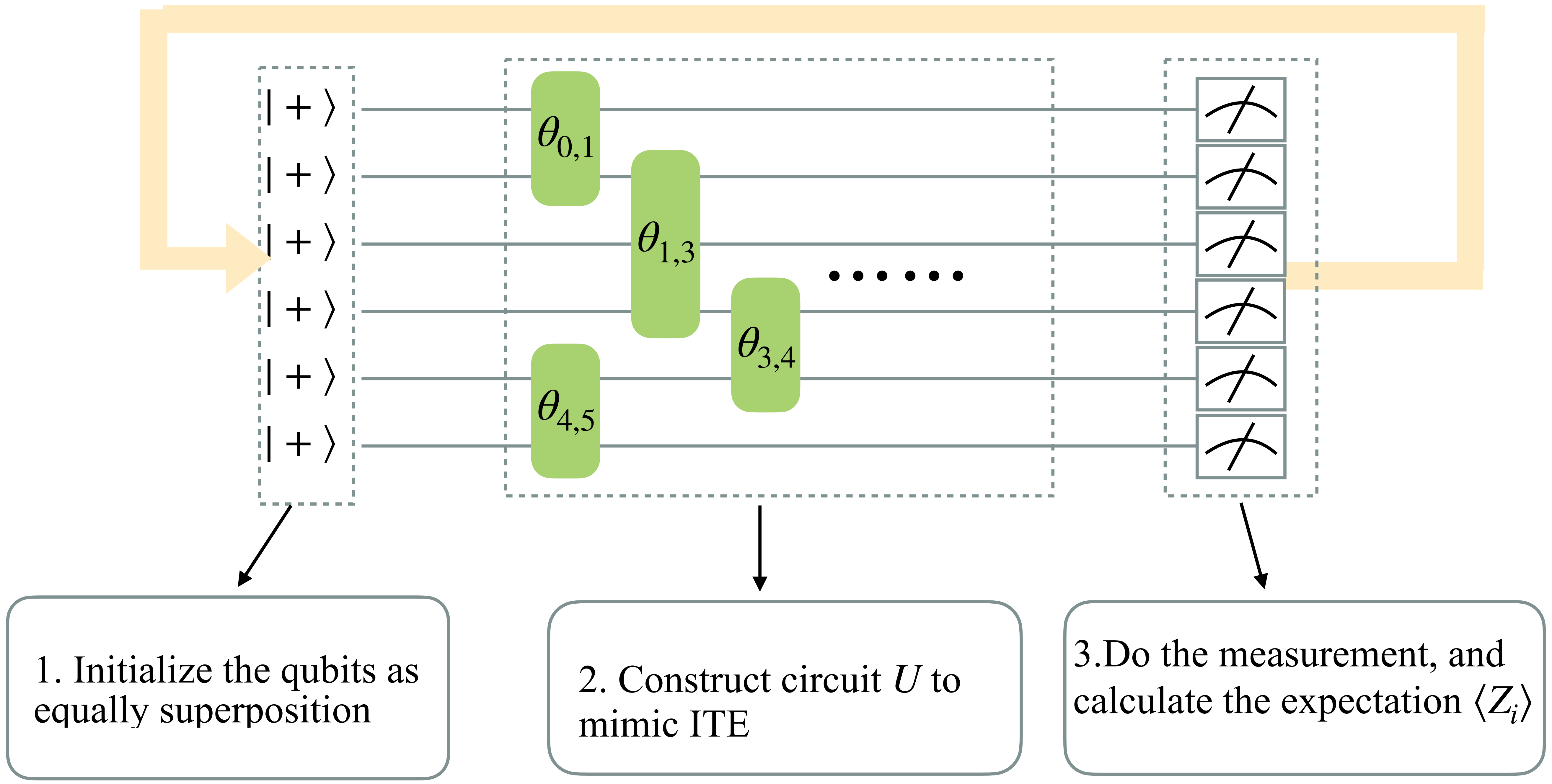
Requirements more practical algorithm…

Shallow circuit with small τ, but iteratively update the initial state

- Physical theorem

$$U|+\rangle^{\otimes N} \sim e^{-\tau \cdot H} \cdot |+\rangle^{\otimes N}$$

- Shallow quantum circuit



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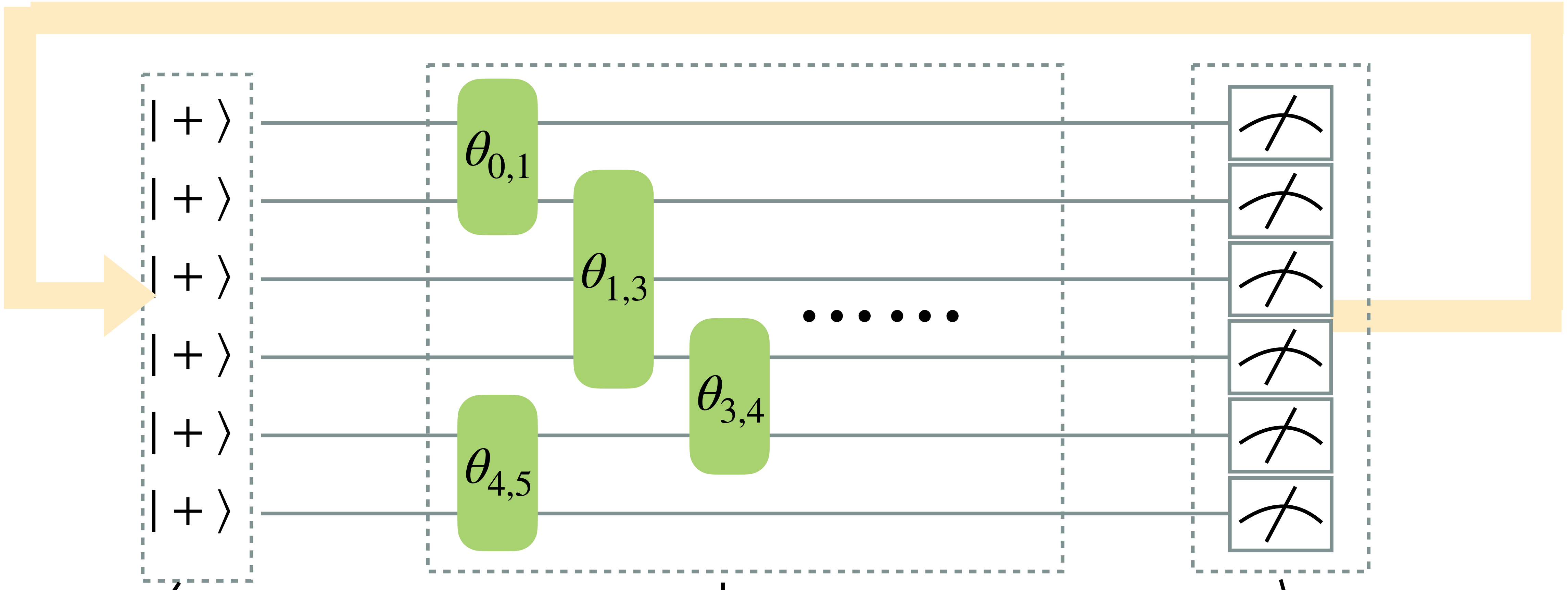

1. Initialize the qubits as equally superposition

2. Construct circuit U to mimic ITE

3.Do the measurement, and calculate the expectation $\langle Z_i \rangle$

$$|+\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

$$\langle +|Z_i|+\rangle = 0$$

$\langle Z_i \rangle > 0$ $\quad |0\rangle \uparrow, \ |1\rangle \downarrow$

$\langle Z_i \rangle < 0$ $\quad |0\rangle \downarrow, \ |1\rangle \uparrow$

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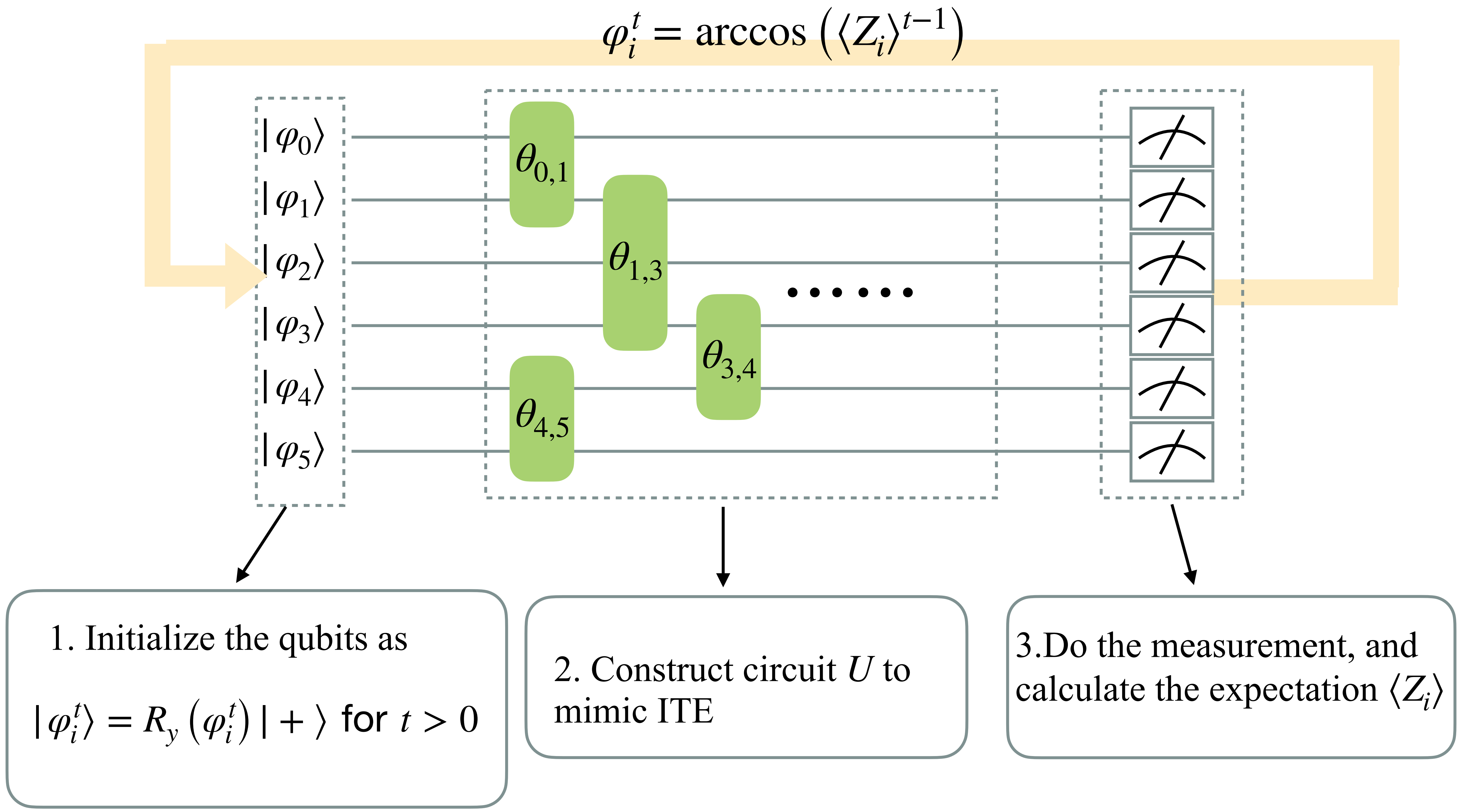

Imaginary time evolution (ITE) of QUBO

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

$$= \prod_{(i,j)} e^{-\tau J_{ij} Z_i Z_j} \times \prod_{i \in V} e^{-\tau h_i Z_i}$$

Mimic ITE using local quantum gate

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Mimic ITE using local quantum gate

Two body term:

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

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

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

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

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

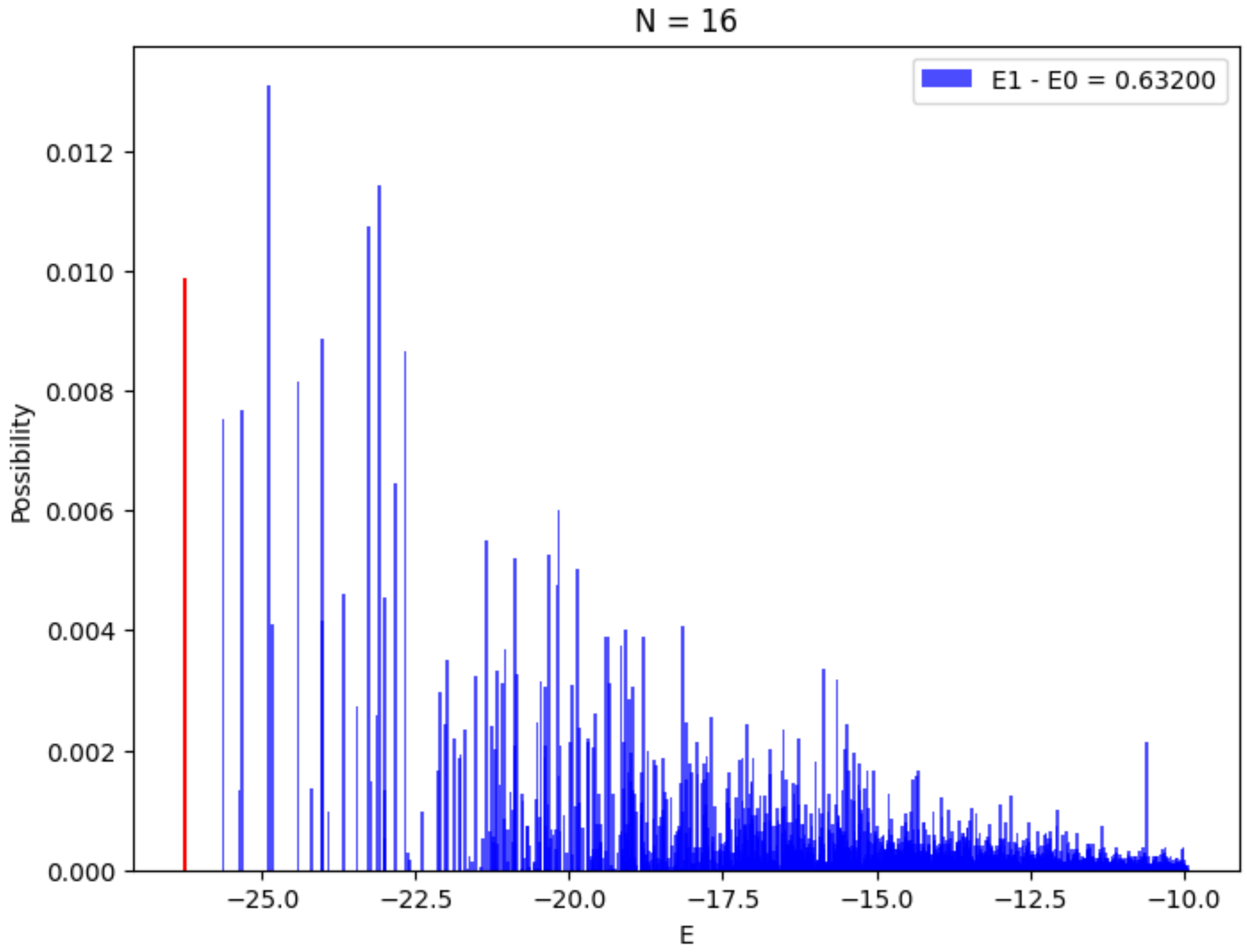
Imaginary time evolution (ITE) of QUBO

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

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

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

$$\vdots$$



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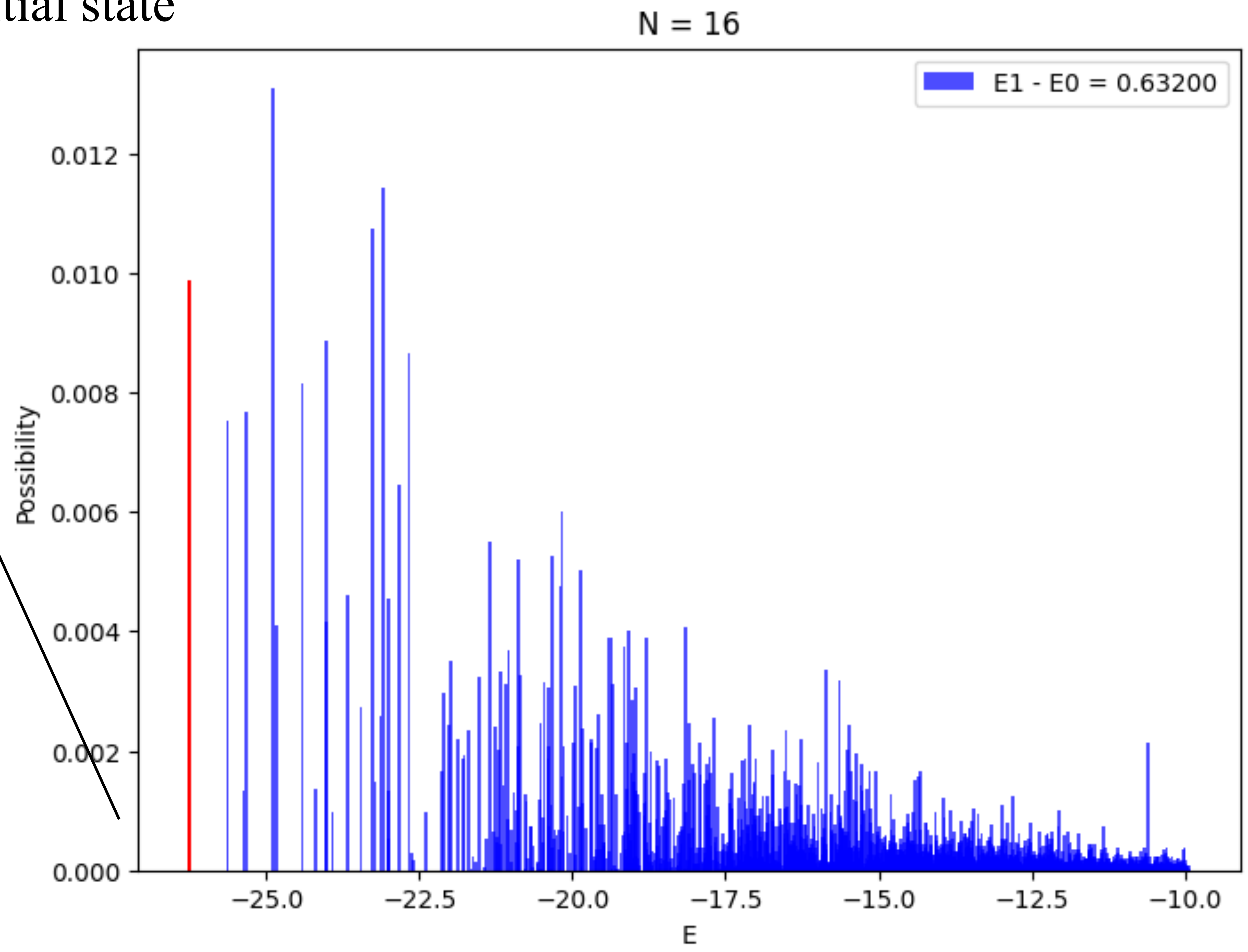
$$|\psi_3\rangle = e^{-i(\alpha_{23}^* Z_2 Y_3 + \beta_{23}^* Y_2 Z_3)/2}\,|\psi_2\rangle$$

$$\vdots$$

Update initial state



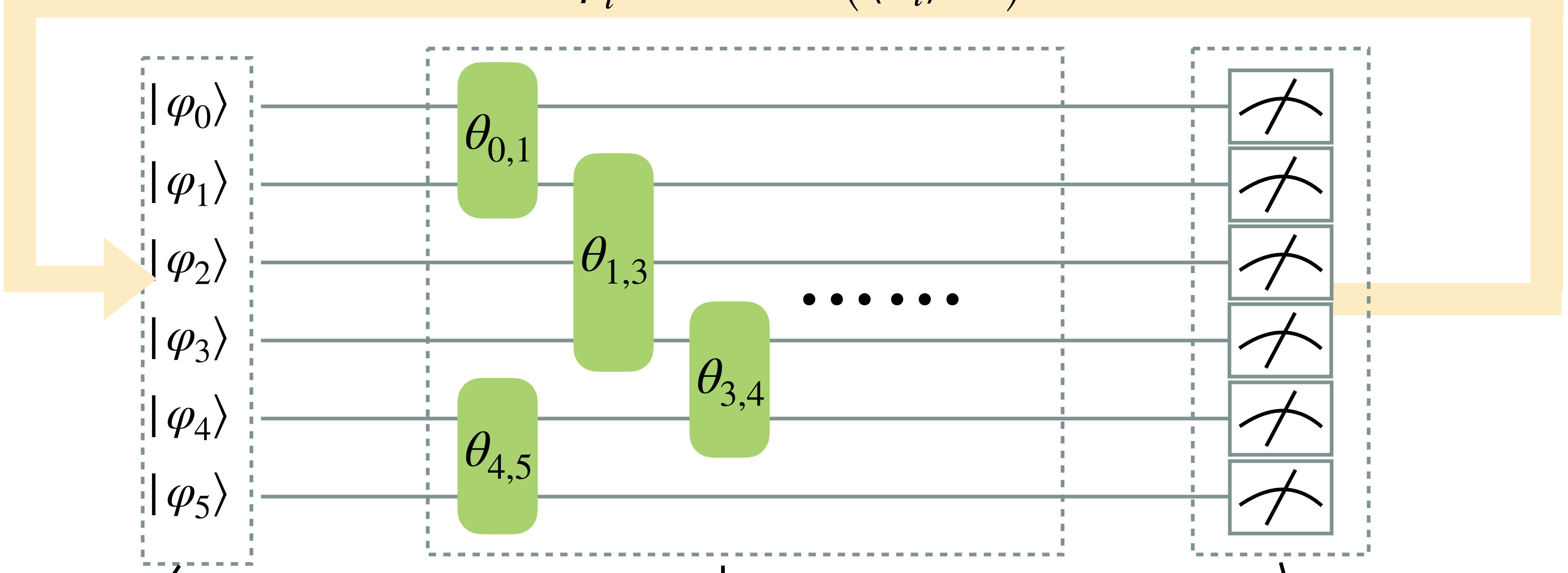
Requirements more practical algorithm…

- Physical theorem
- Shallow quantum circuit
- **Fewer measurements**

Shallow circuit with small τ, but iteratively update the initial state

$$U|+\rangle^{\otimes N} \sim e^{-\tau \cdot H} \cdot |+\rangle^{\otimes N}$$

$$\varphi_i^t = \arccos\left(\langle Z_i \rangle^{t-1}\right)$$



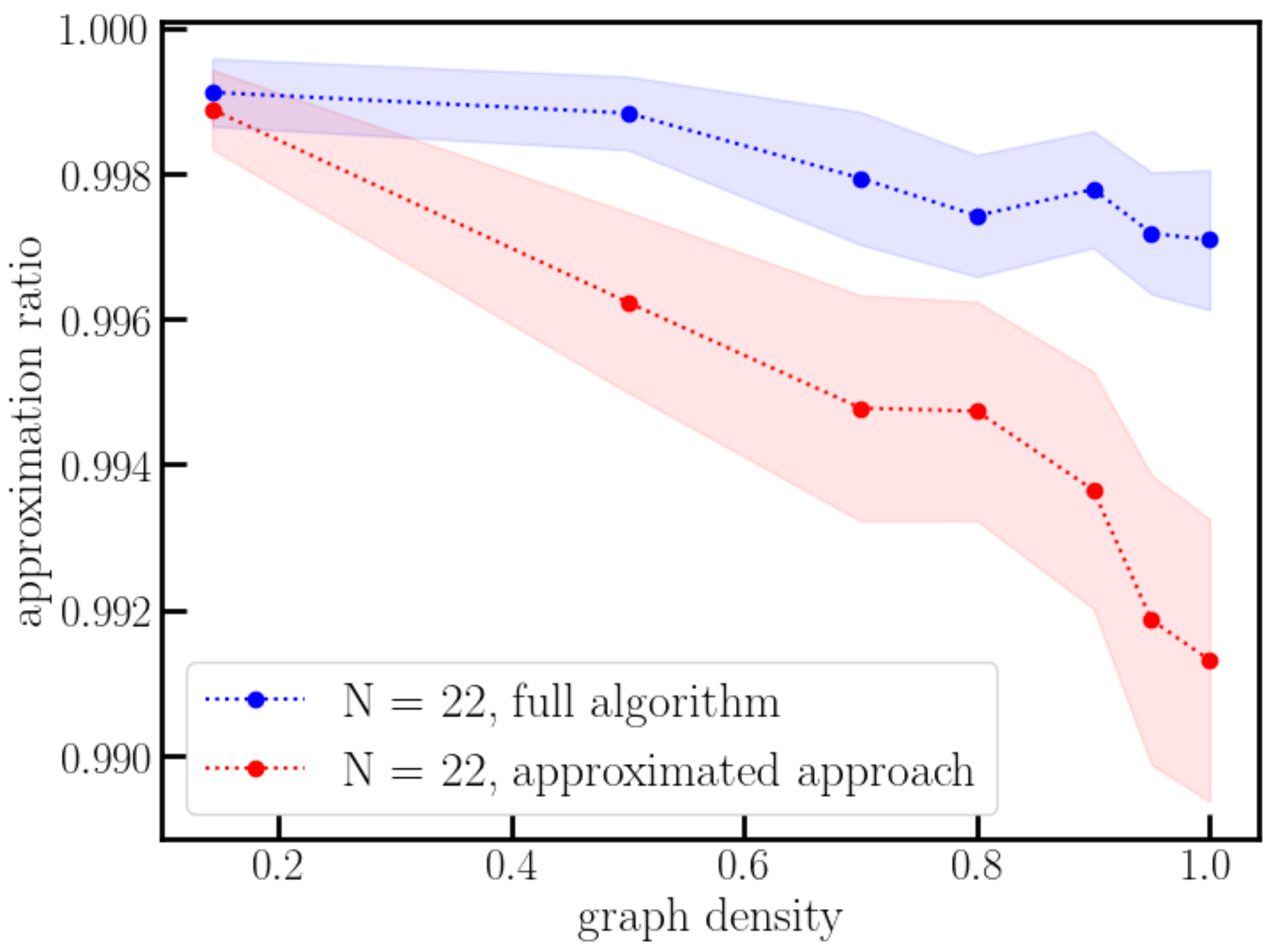
1. Initialize the qubits as $|\varphi_i^t\rangle = R_y\left(\varphi_i^t\right)|+\rangle$ for $t > 0$

2. Construct circuit U to mimic ITE

3. Do the measurement, and calculate the expectation $\langle Z_i \rangle$

Only need the expectation of one- and two-qubit operators

Classical simulation Results



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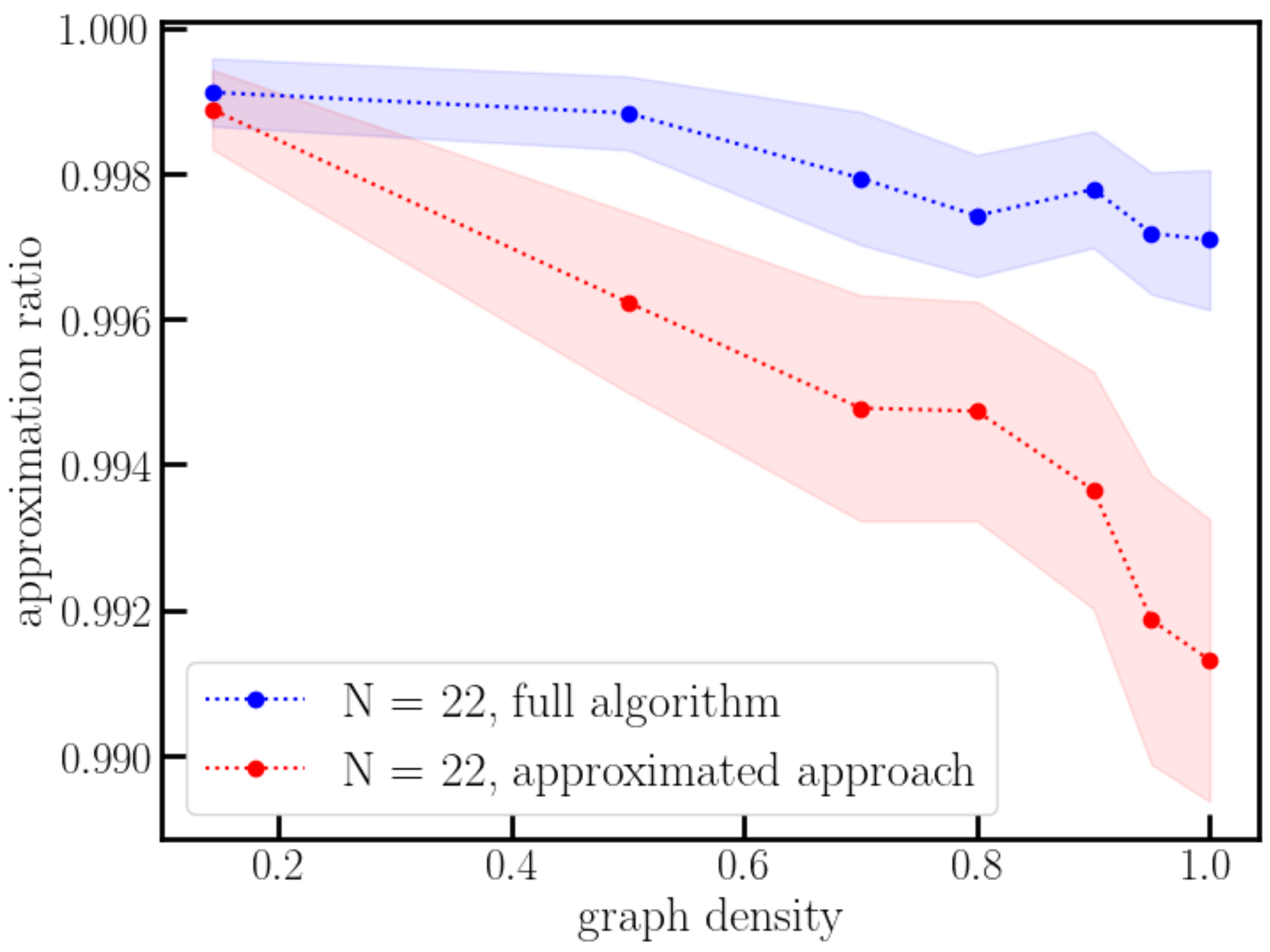

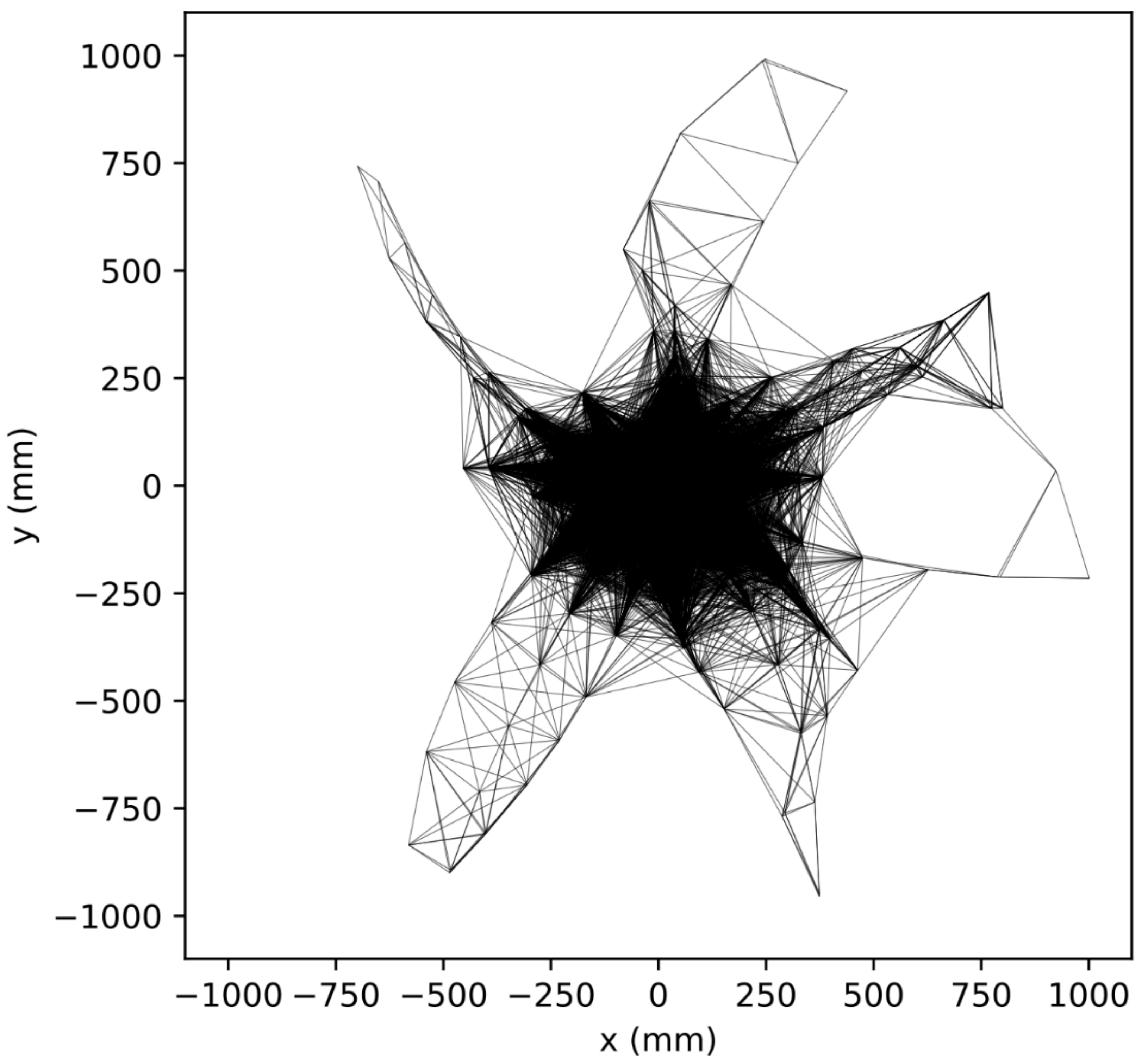

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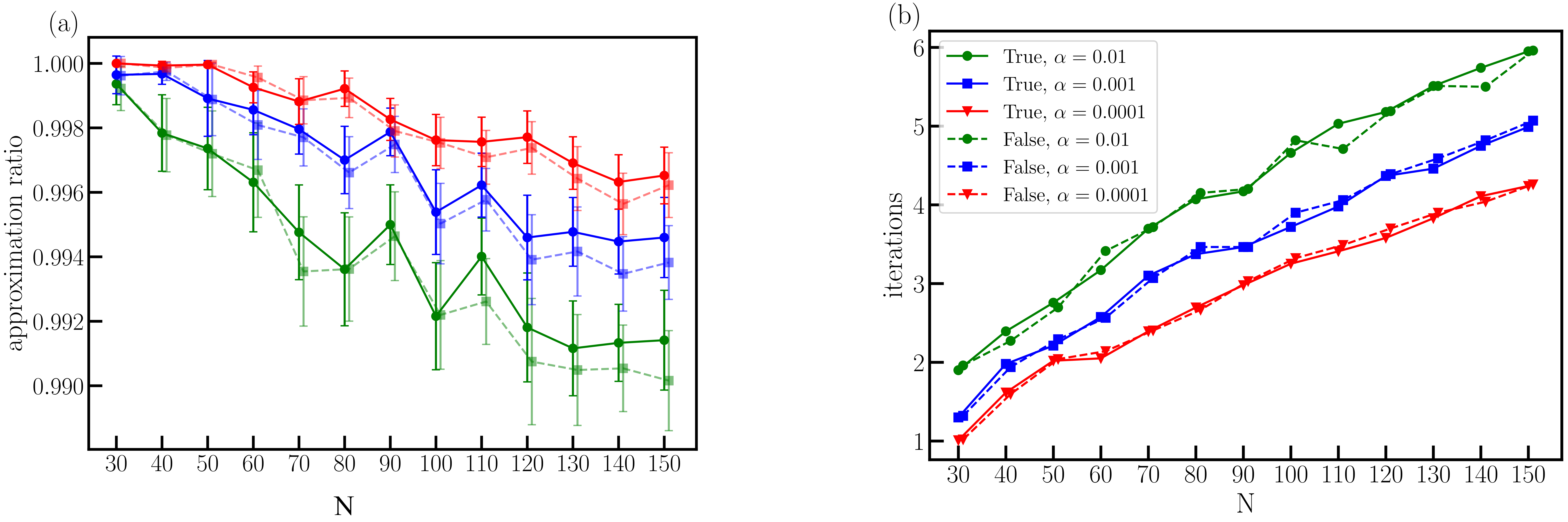
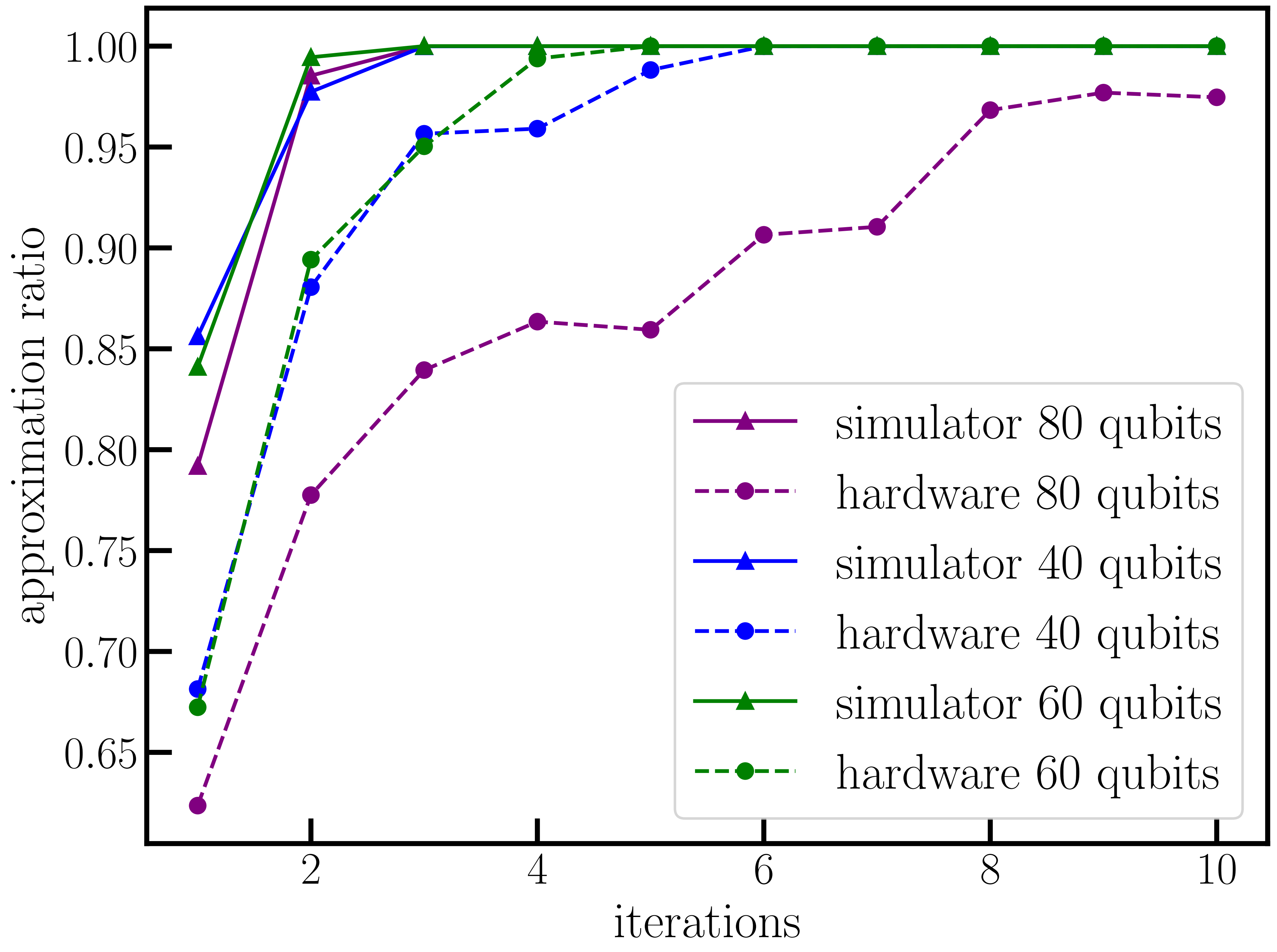


Hardware run on IBM device



Two-qubit depth: 45, 55, 65 for 40, 60, 80 qubits

Summary and outlook

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  - Map particle tracking to QUBO problem
  - ITEMC algorithm for solving QUBO. Successfully executed hardware run upto 80 qubits

- Outlook
  - Improved modeling of particle tracking
  - Different encoding?
  - Improved initial state update
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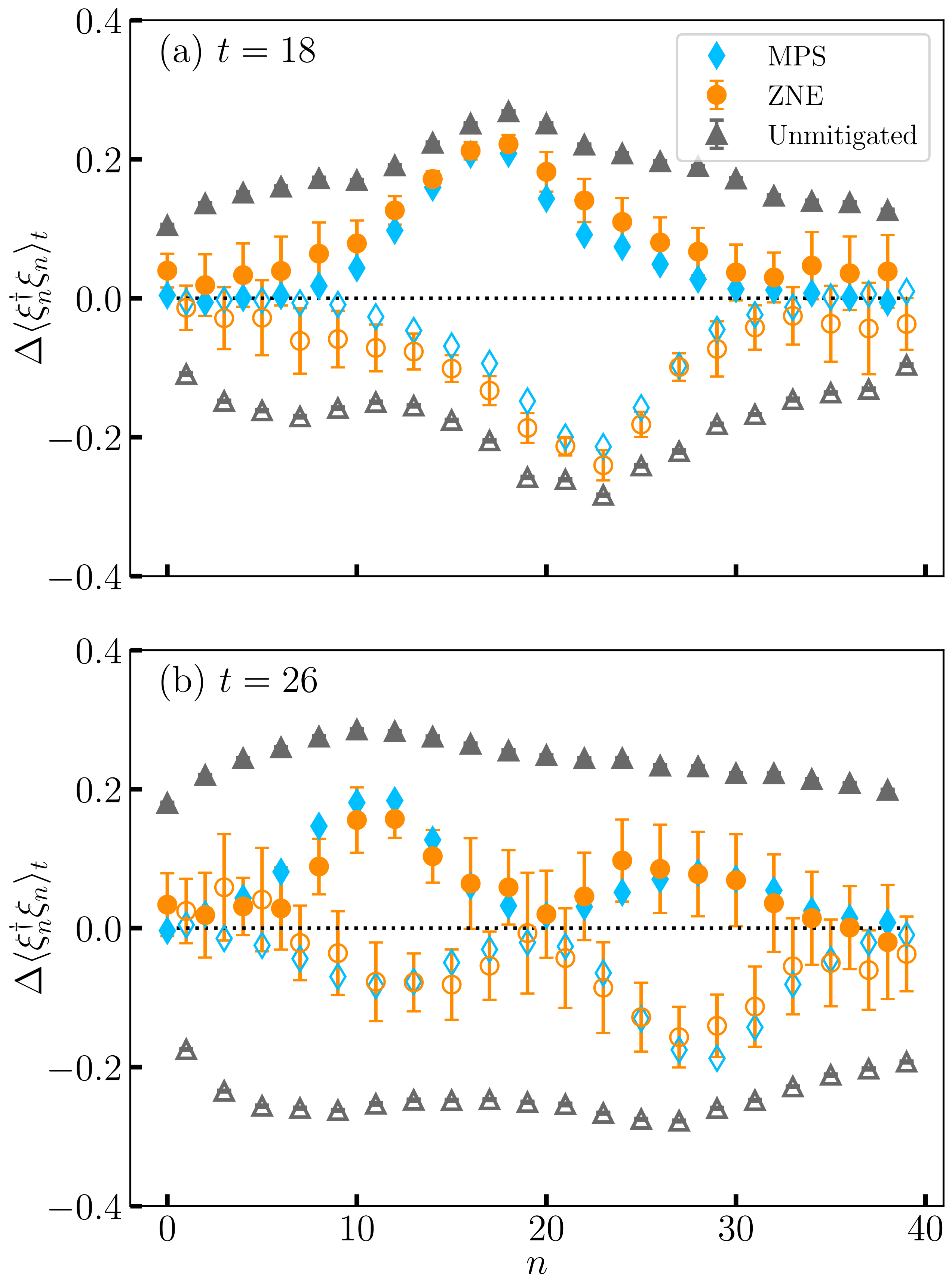

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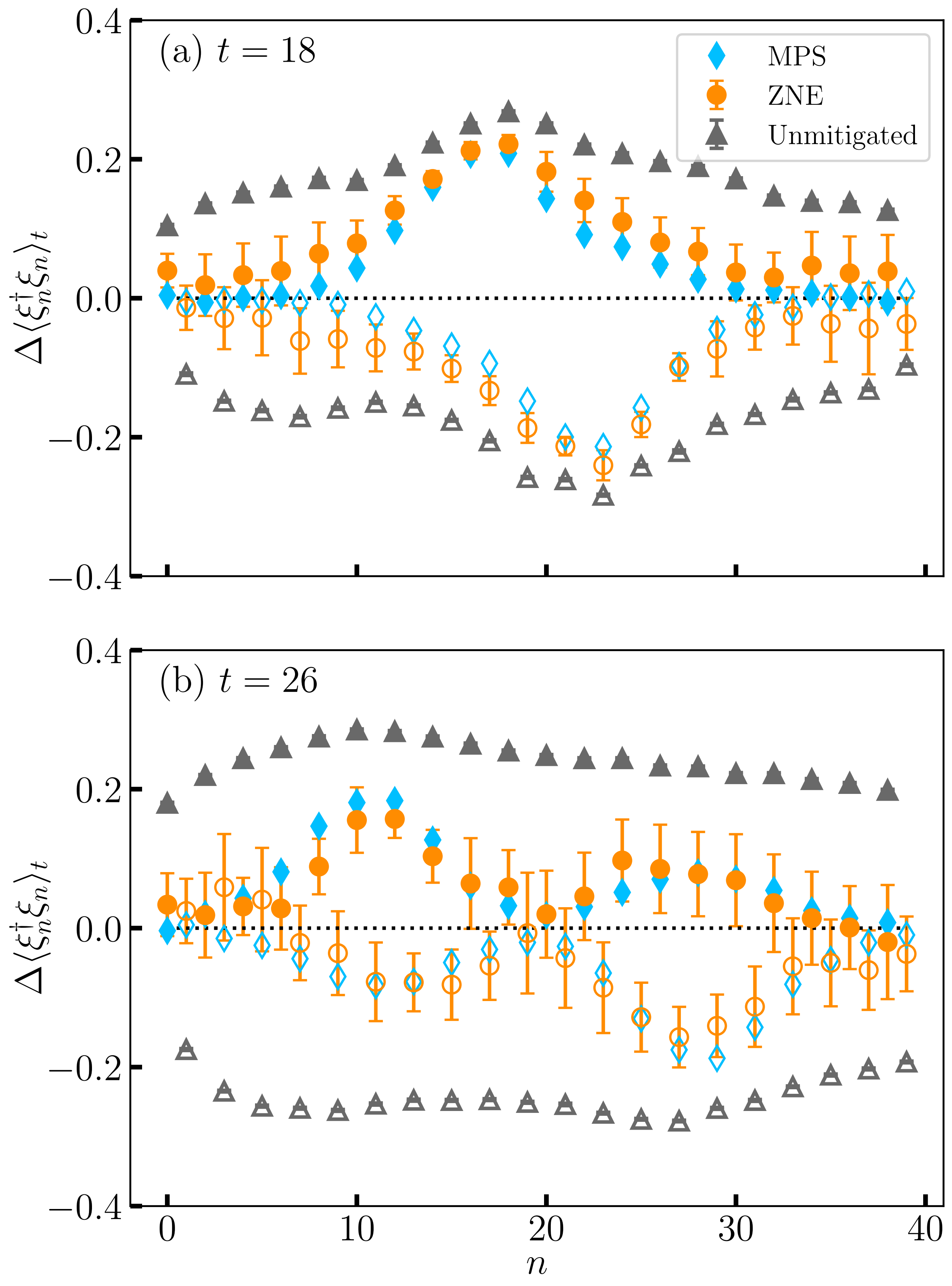

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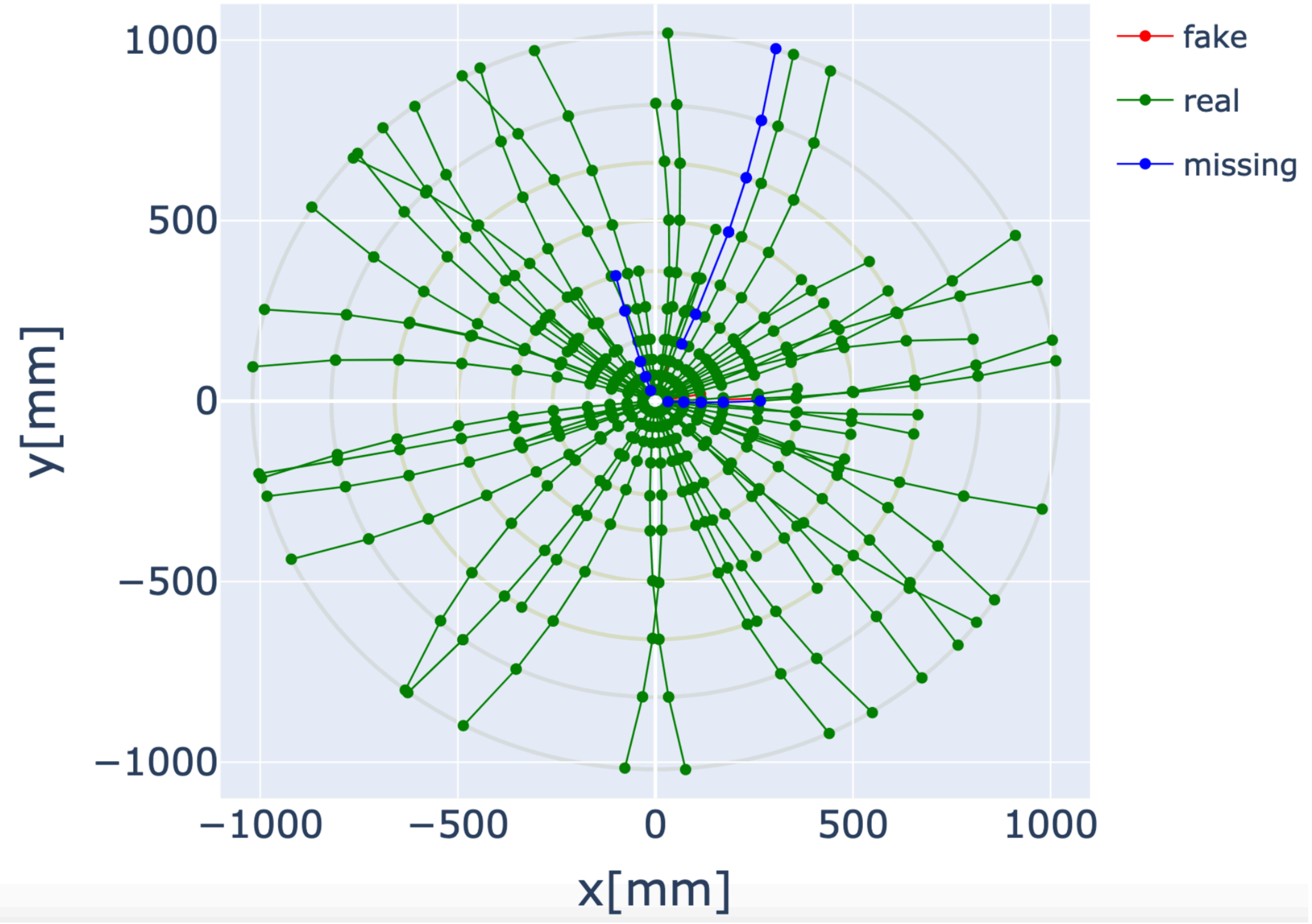
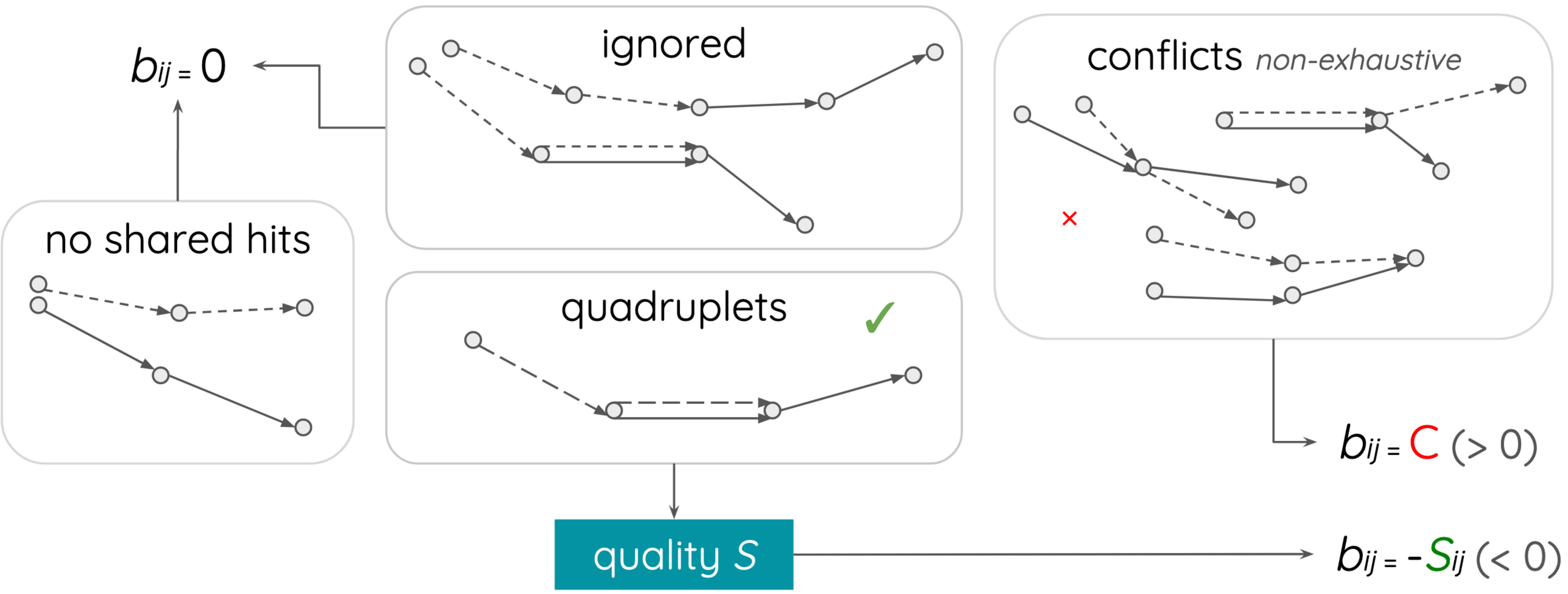
Thanks!

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.

Particle tracking

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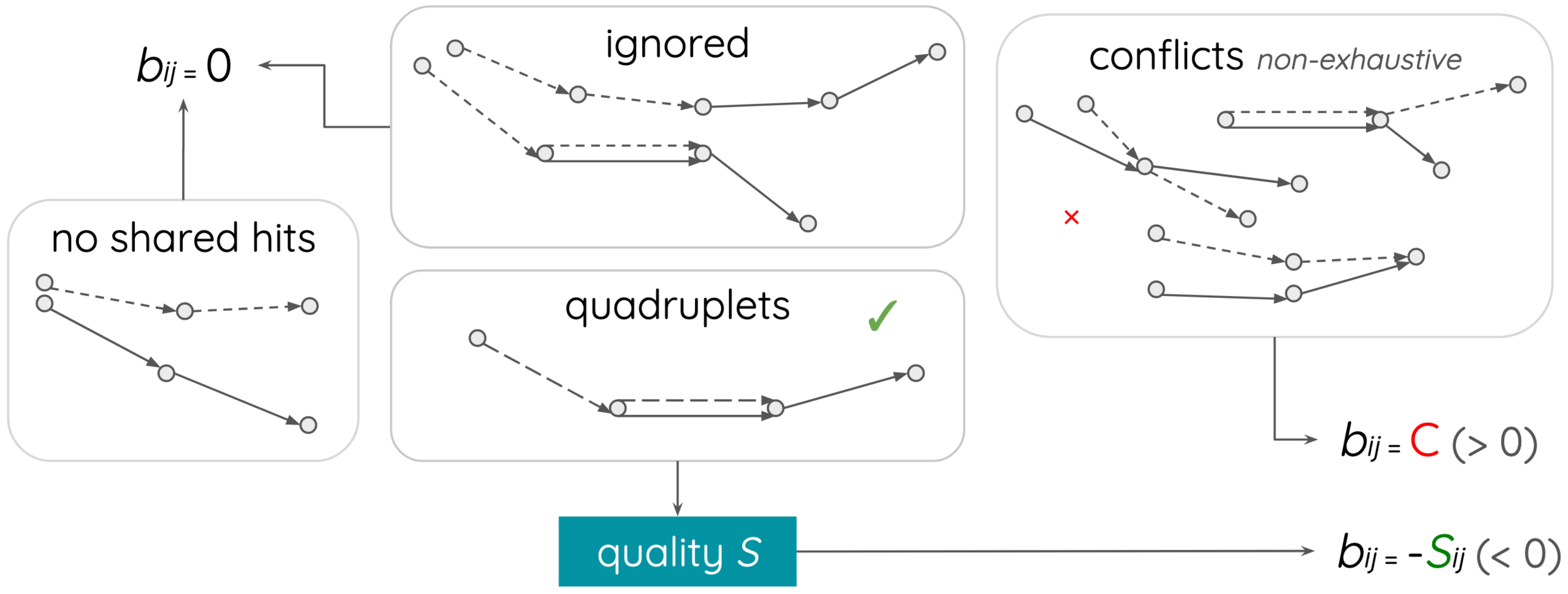
- Construct QUBO cost function

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

  - 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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