Enhancing Quantum Utility: Simulating Large-scale Quantum Spin Chains on Superconducting Quantum Computers

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Introduction

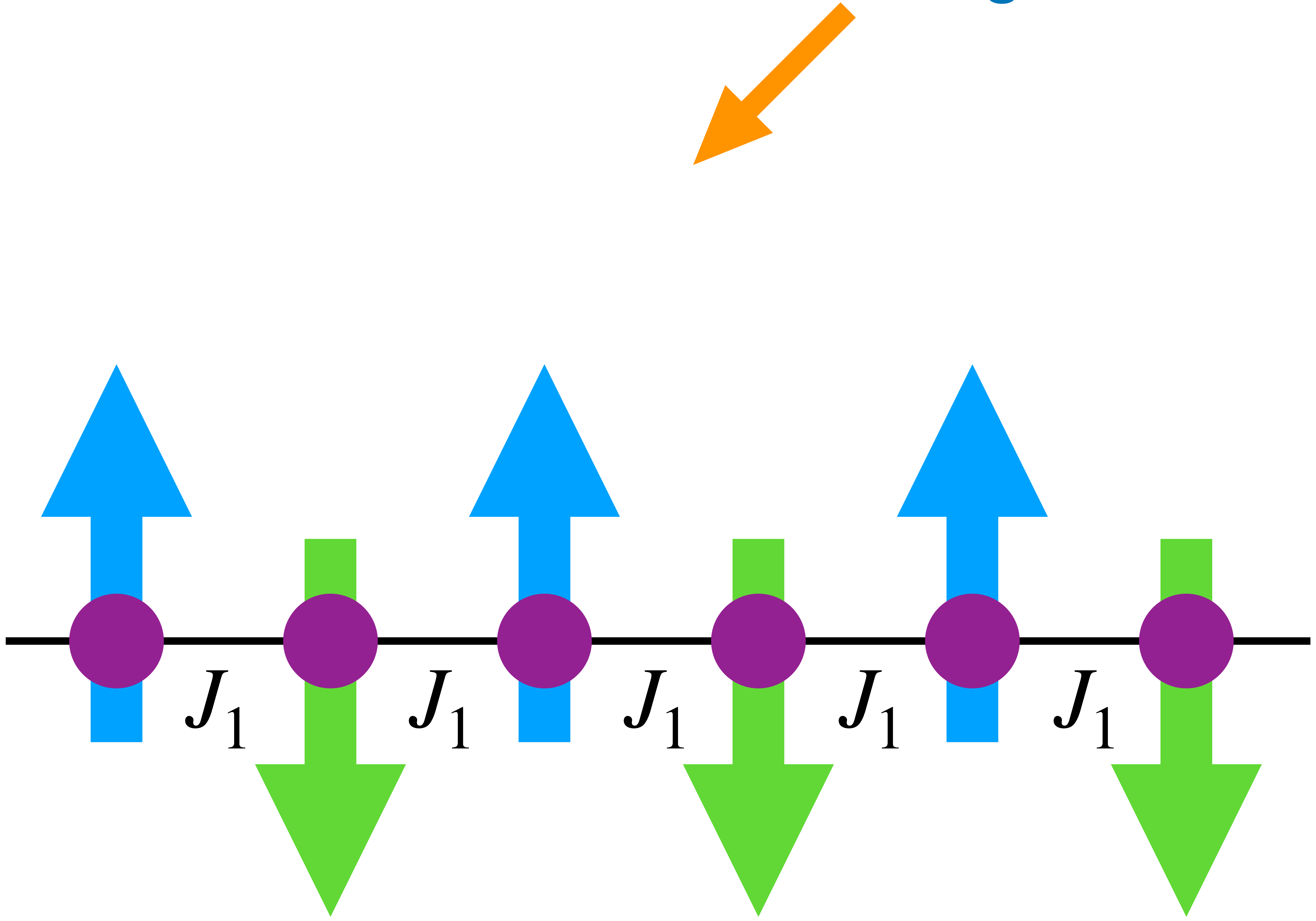
- Quantum computing is a rapidly evolving field.
- Significant development in this field has led to the emergence of Noisy Quantum computers.
- Can we utilize these real quantum computers to study fundamental physics?
- Require rigorous testing, validation and benchmarking well-established results in current real quantum hardwares.
- Our work explored if current noisy quantum computer is capable enough to capture the real-time dynamics of large-scale quantum many-body system.

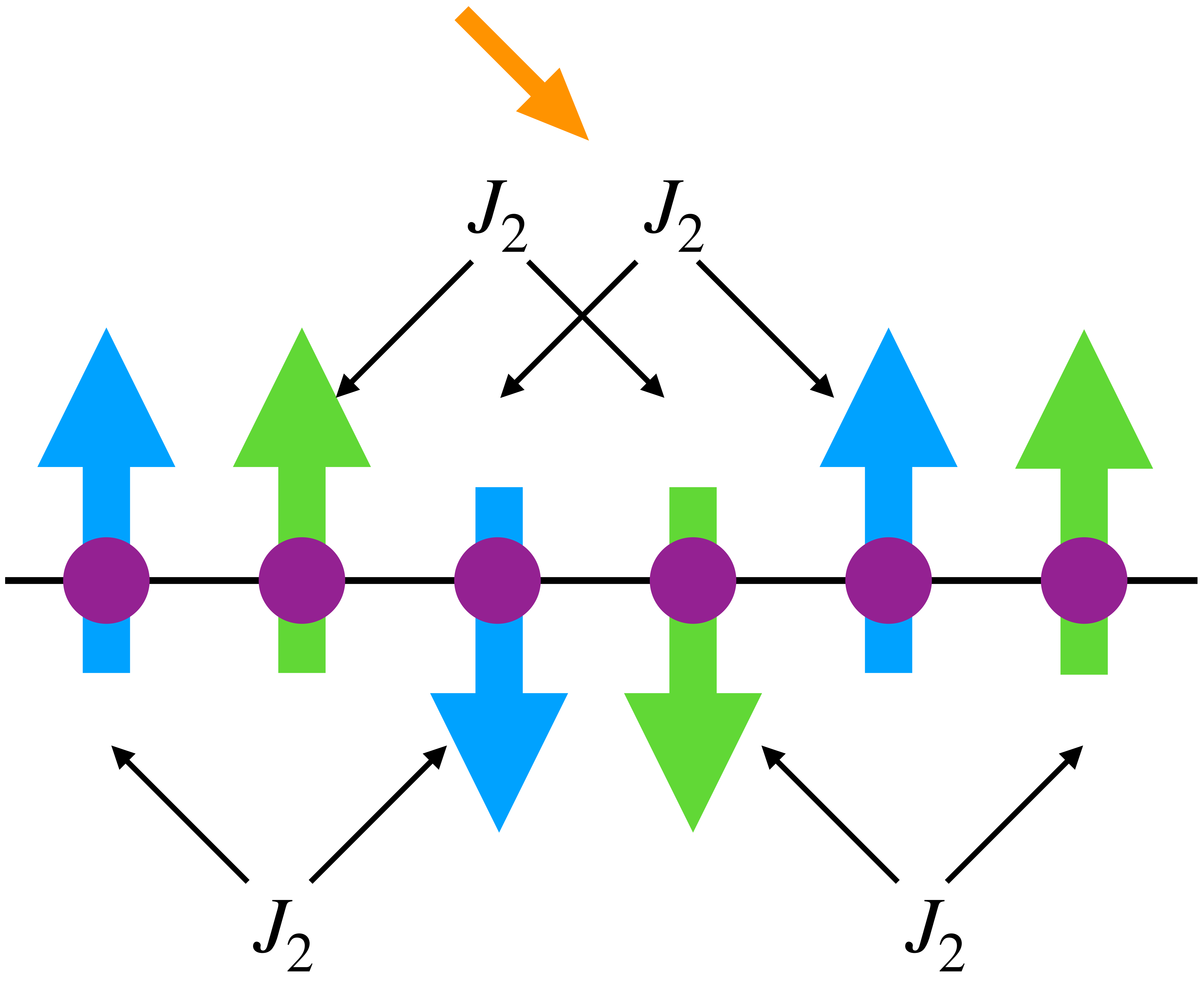
Frustrated spin-$\frac{1}{2}$ antiferromagnetic spin chain model ($J_1 - J_2$ model)

$$H = J_1 \sum_{i=1}^{N-1} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta\, S_i^z S_{i+1}^z \right) + J_2 \sum_{i=1}^{N-2} \left(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + S_i^z S_{i+2}^z \right)$$

Nearest-Neighbor

Next-Nearest-Neighbor





Haldane, Phys.Rev.B, 25, 4925 (1982)

Real-time Dynamics in $J_1 - J_2$ model

- For time-independent Hamiltonian, the time-evolved state is given by $|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle$

- We focused on time evolution of an observable $\hat{O}$ with respect to time-evolved state $|\psi(t)\rangle$ as $\langle\psi(t)|\hat{O}|\psi(t)\rangle$

- Our initial state is Neel state $|\psi_{\text{Neel}}(0)\rangle = |\uparrow\downarrow\uparrow\downarrow\ldots\uparrow\downarrow\rangle$

- For the observable we chose the staggered magnetization which captures the antiferromagnetic ordering

$$\hat{O}_{M_{st}} = \frac{1}{N}\sum_{i=1}^{N}(-1)^i S_i^z$$

Real-time Dynamics in $J_1 - J_2$ model

- We choose two Hamiltonians for our real-time dynamics in $J_1 - J_2$ model:

$$H = J_1 \sum_{i=1}^{N-1} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta\, S_i^z S_{i+1}^z \right) + J_2 \sum_{i=1}^{N-2} \left(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + S_i^z S_{i+2}^z \right)$$

$\Delta = 1, J_2 = 0$ $\quad$ $\Delta = 1, J_2 = J_1/2$

$$H_{\text{iso}} = J_1 \sum_{i=1}^{N-1} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z \right)$$

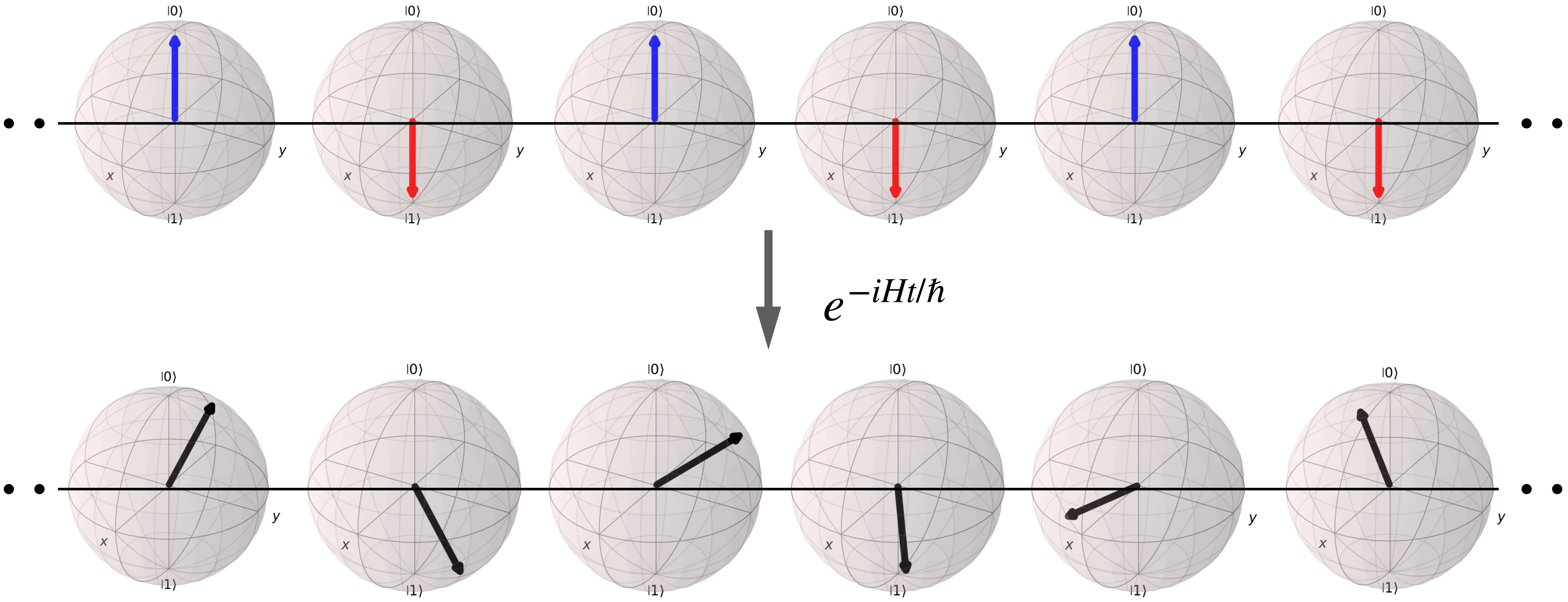
Isotropic Heisenberg Hamiltonian

$$H_{\text{Dimer}} = J_1 \sum_{i=1}^{N-1} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z \right) + \frac{J_1}{2} \sum_{i=1}^{N-2} \left(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + S_i^z S_{i+2}^z \right)$$

Dimer Hamiltonian

- $|\psi_{\text{Neel}}\rangle$ is not an eigenstate of either H_{iso} or H_{Dimer} so non-trivial time evolution will take place.

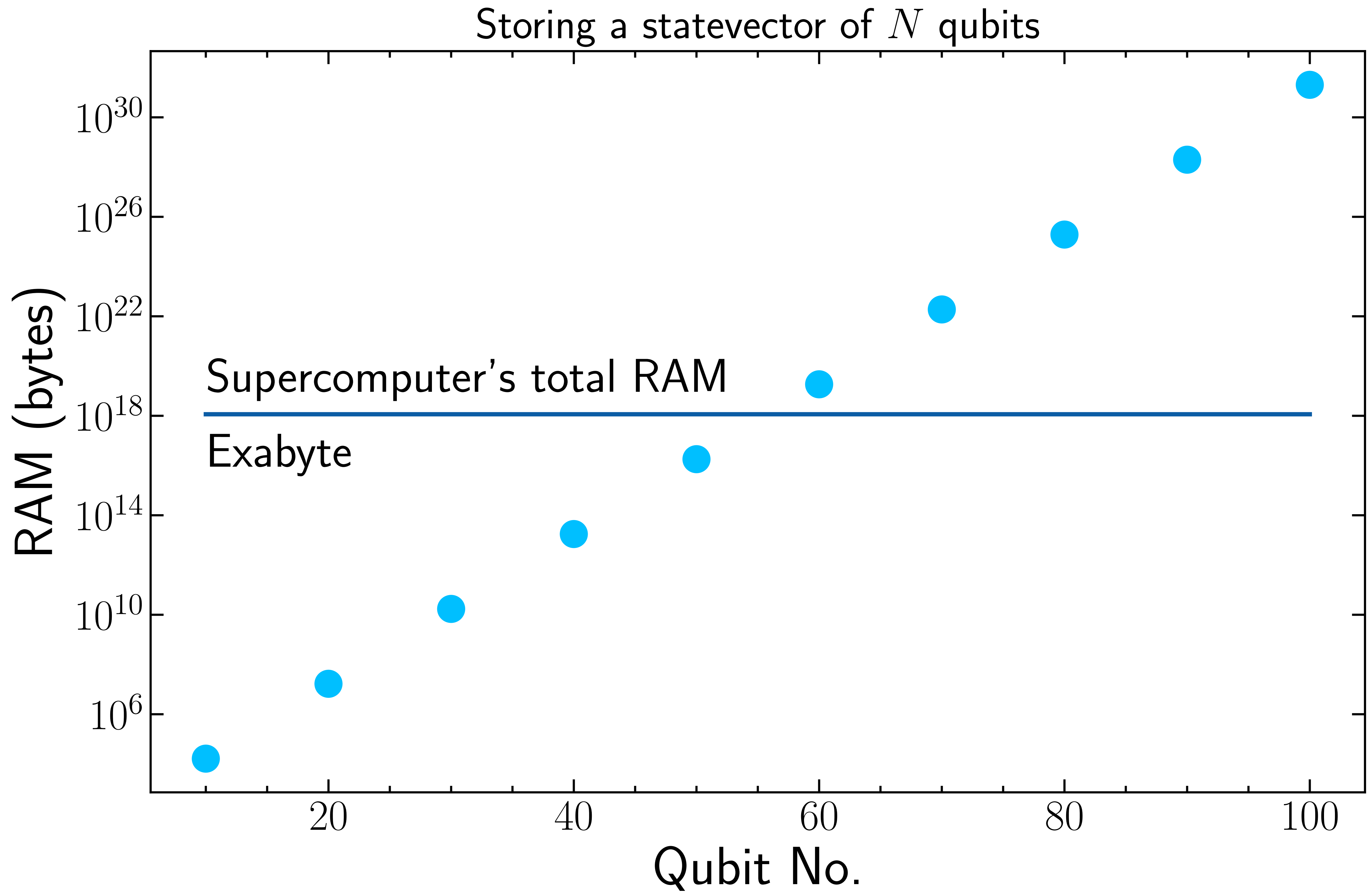
Real-time Dynamics in $J_1 - J_2$ model



Relaxation of antiferromagnetic ordering is captured by $\langle \psi(t) \,|\, \hat{O}_{M_{st}} \,|\, \psi(t) \rangle$

Capturing Spin Dynamics in large-scale spin chain

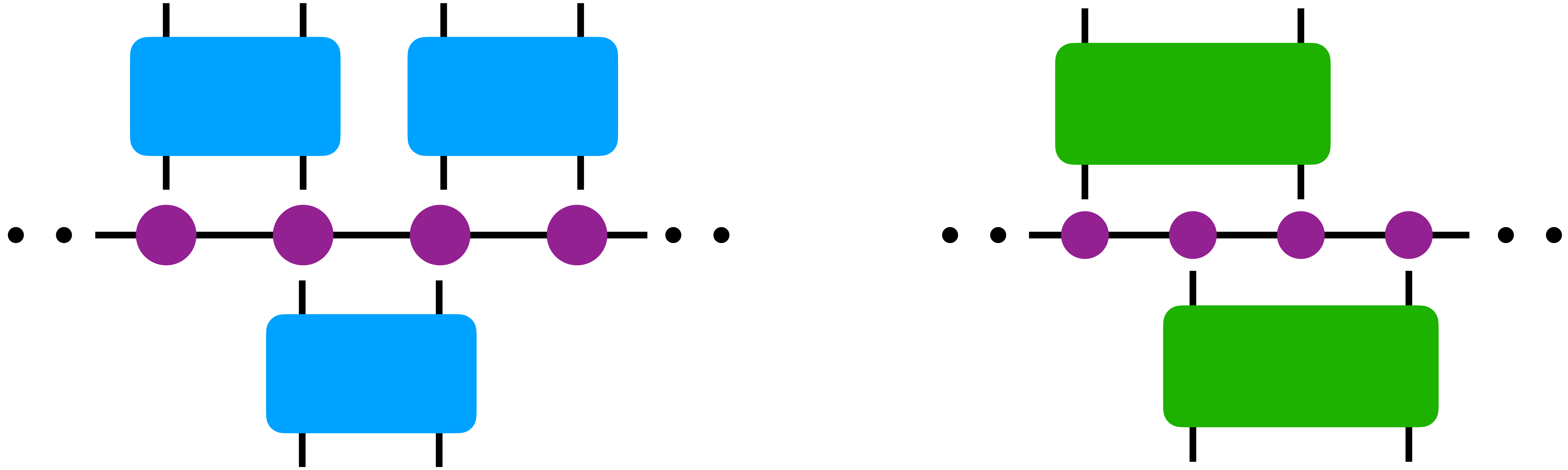
- We can compute explicitly $|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle$
- If the spin-chain has N spin-1/2 particles (qubits), we need to store the statevector $|\psi\rangle \in \mathbb{C}^{2^N}$ in memory.



- The memory requirement to store $|\psi\rangle$ scales exponentially.

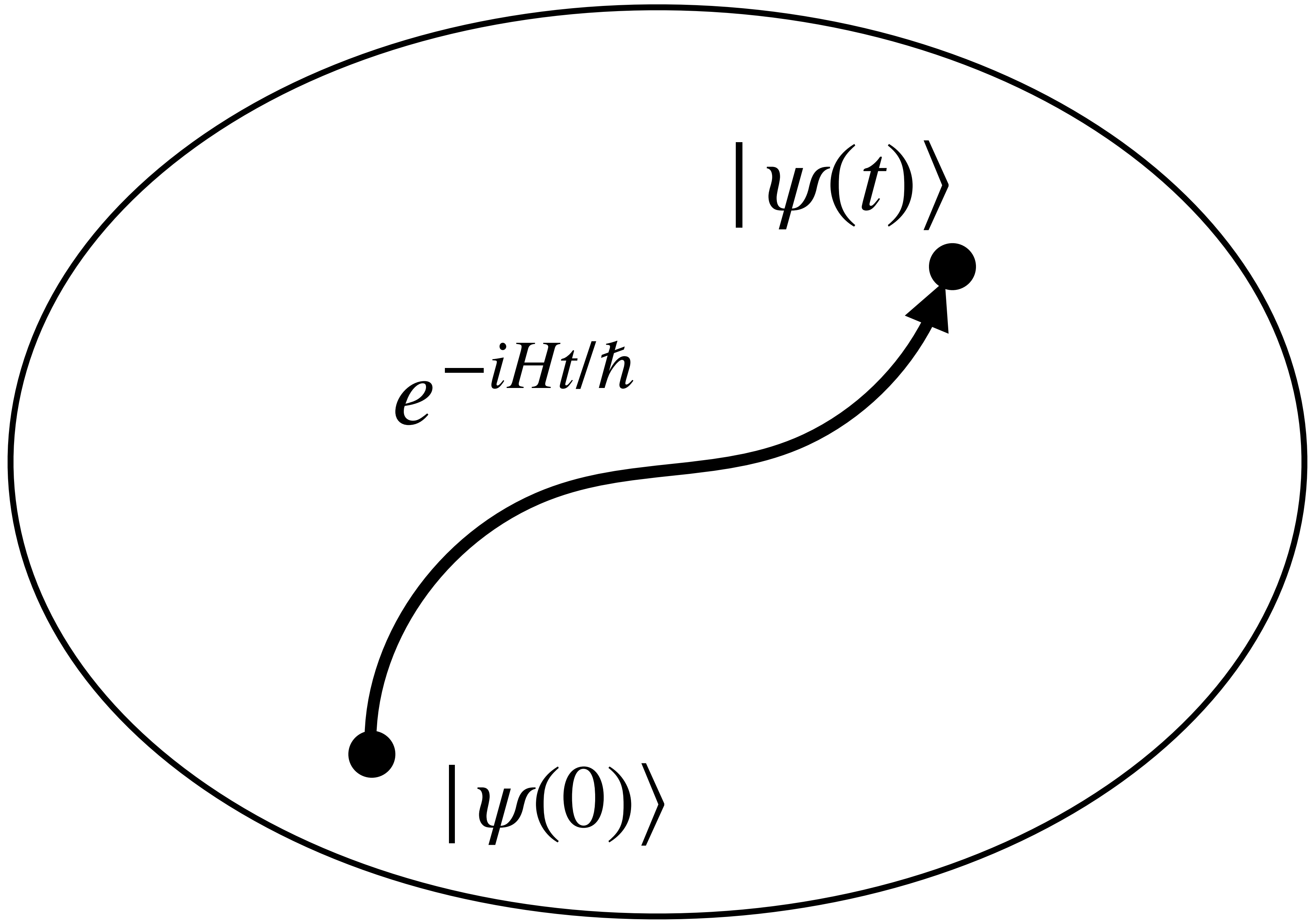
Time Evolution in Quantum Computers

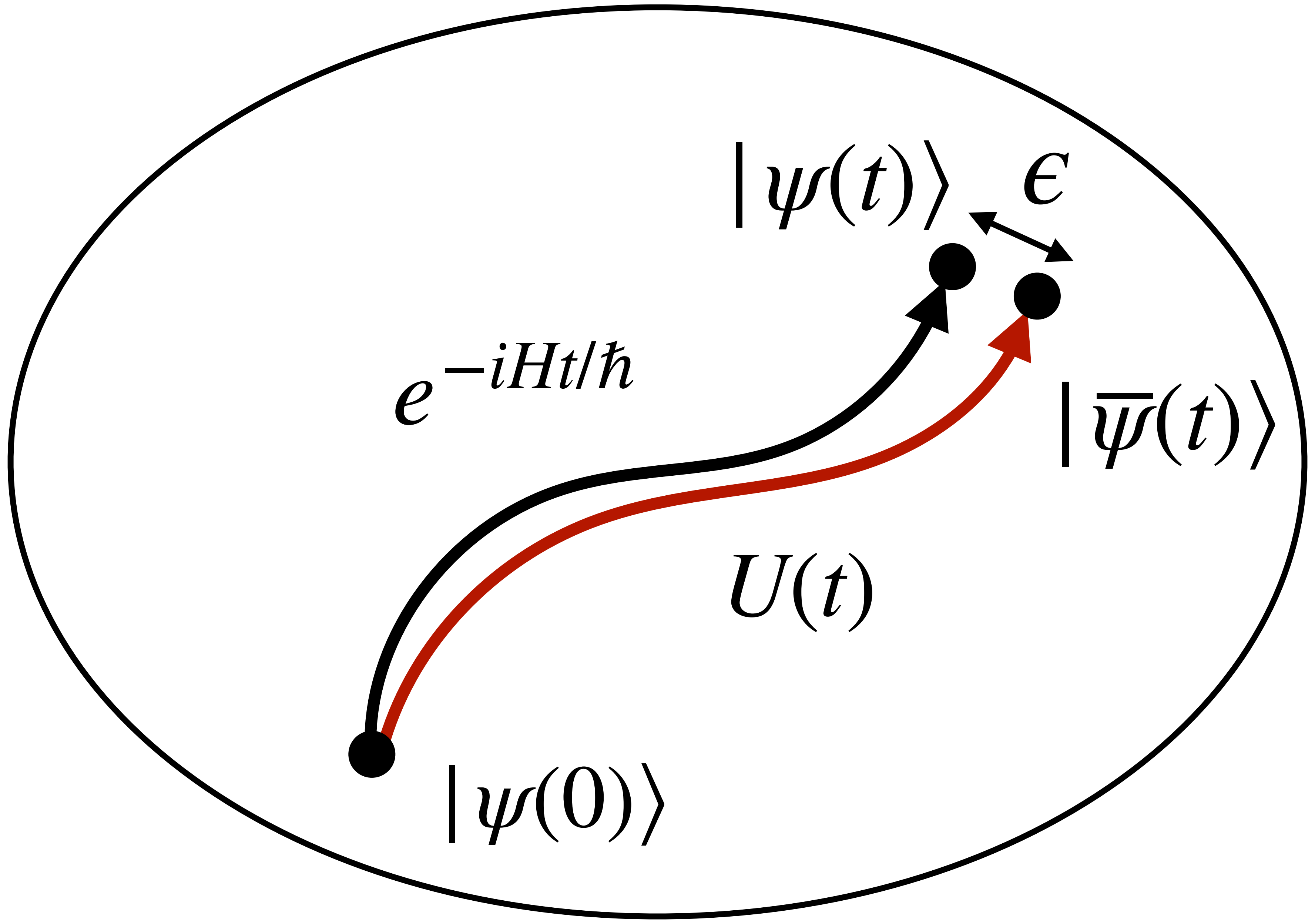
- The Hamiltonian contains L terms, $H = \sum_{j=1}^{L} H_j$



Time evolution operator, $e^{-iHt/\hbar} = e^{-i(H_1 + \ldots + H_L)t/\hbar}$

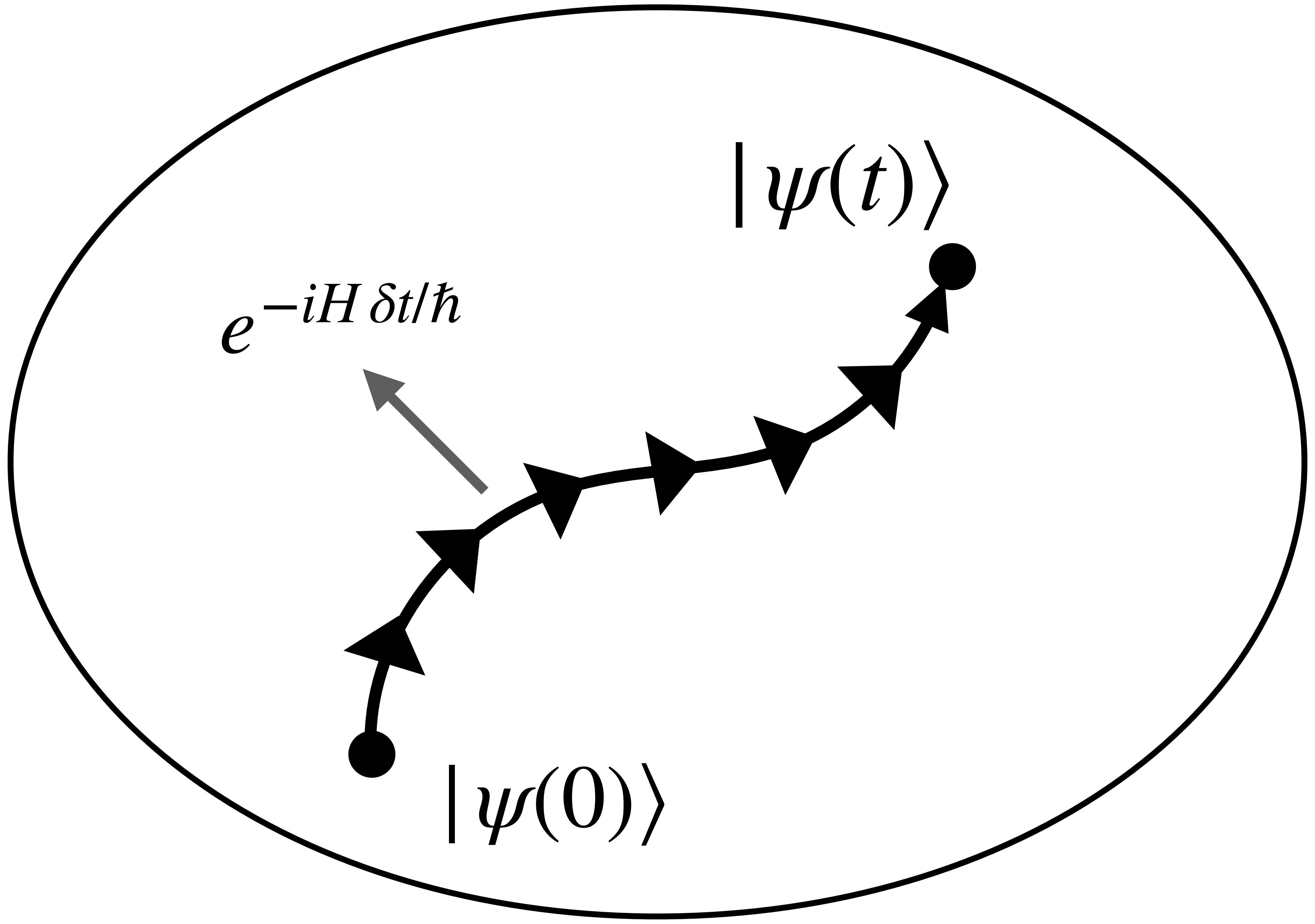
Time Evolution in Quantum Computers

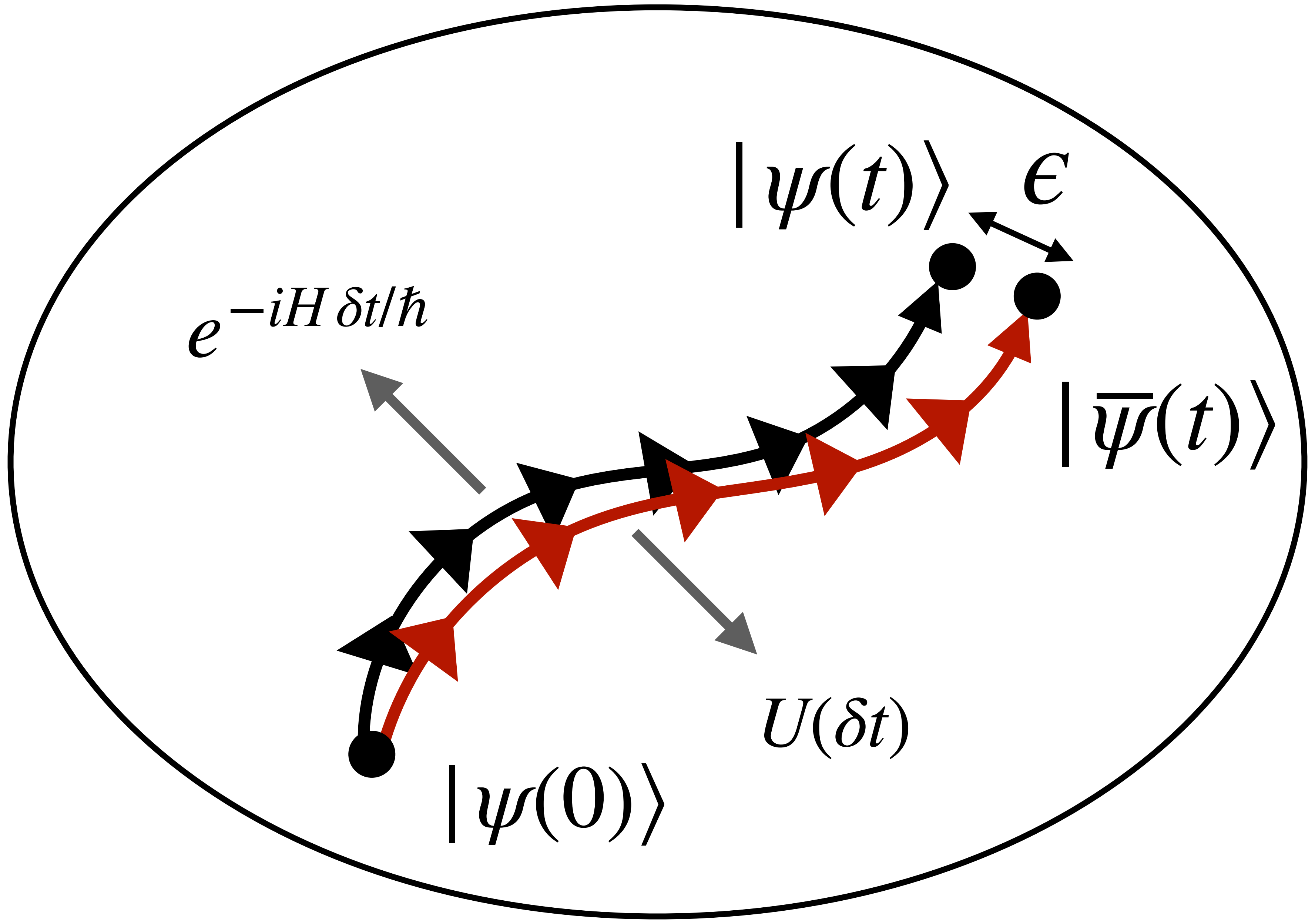




$$|| \, |\psi(t)\rangle - |\overline{\psi}(t)\rangle \, || < \epsilon$$

Time Evolution in Quantum Computers: Trotterization





Time interval t is divided into m intervals of duration $\delta t = t/m$

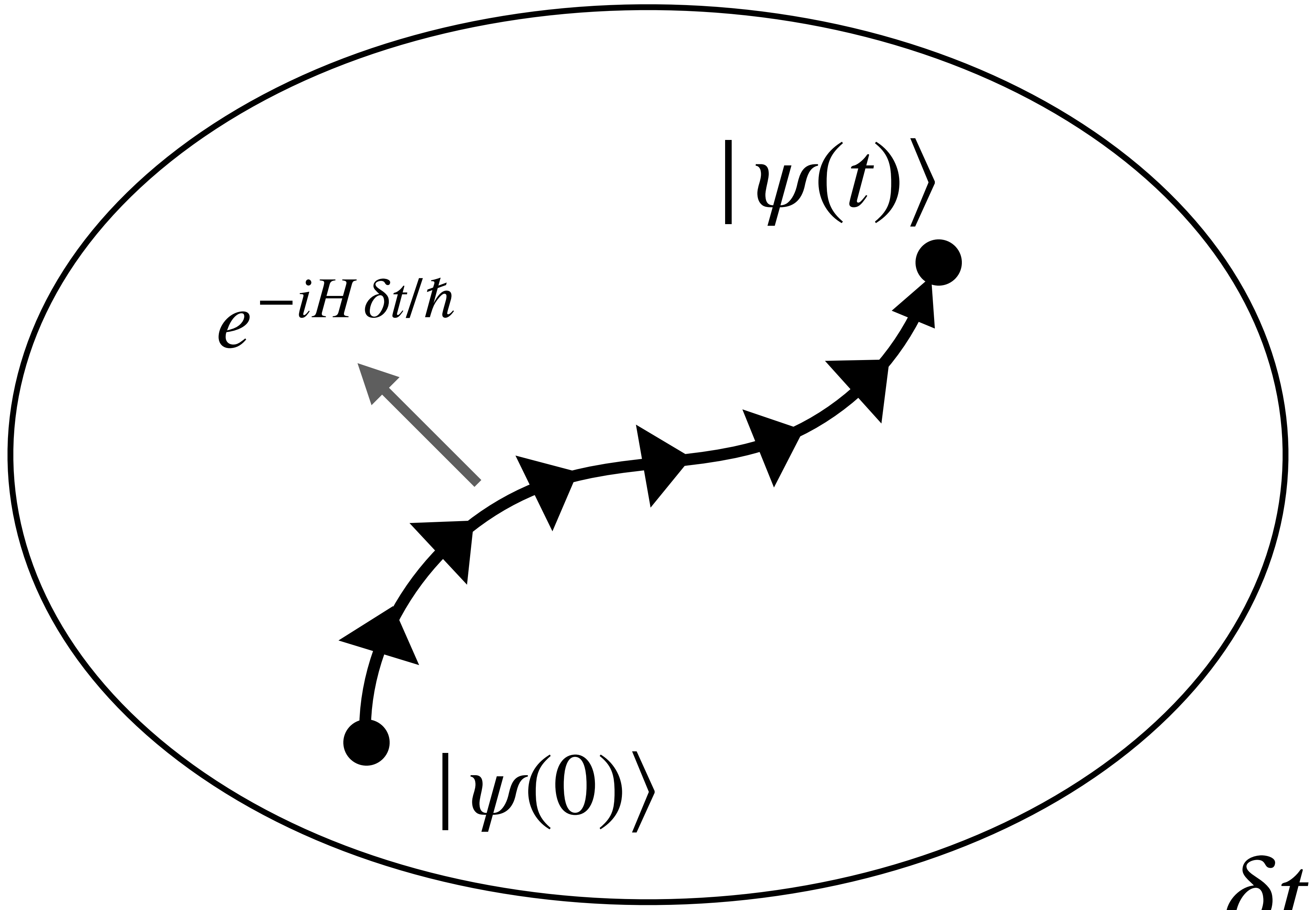
$$U(t) = \prod_m U(\delta t)$$

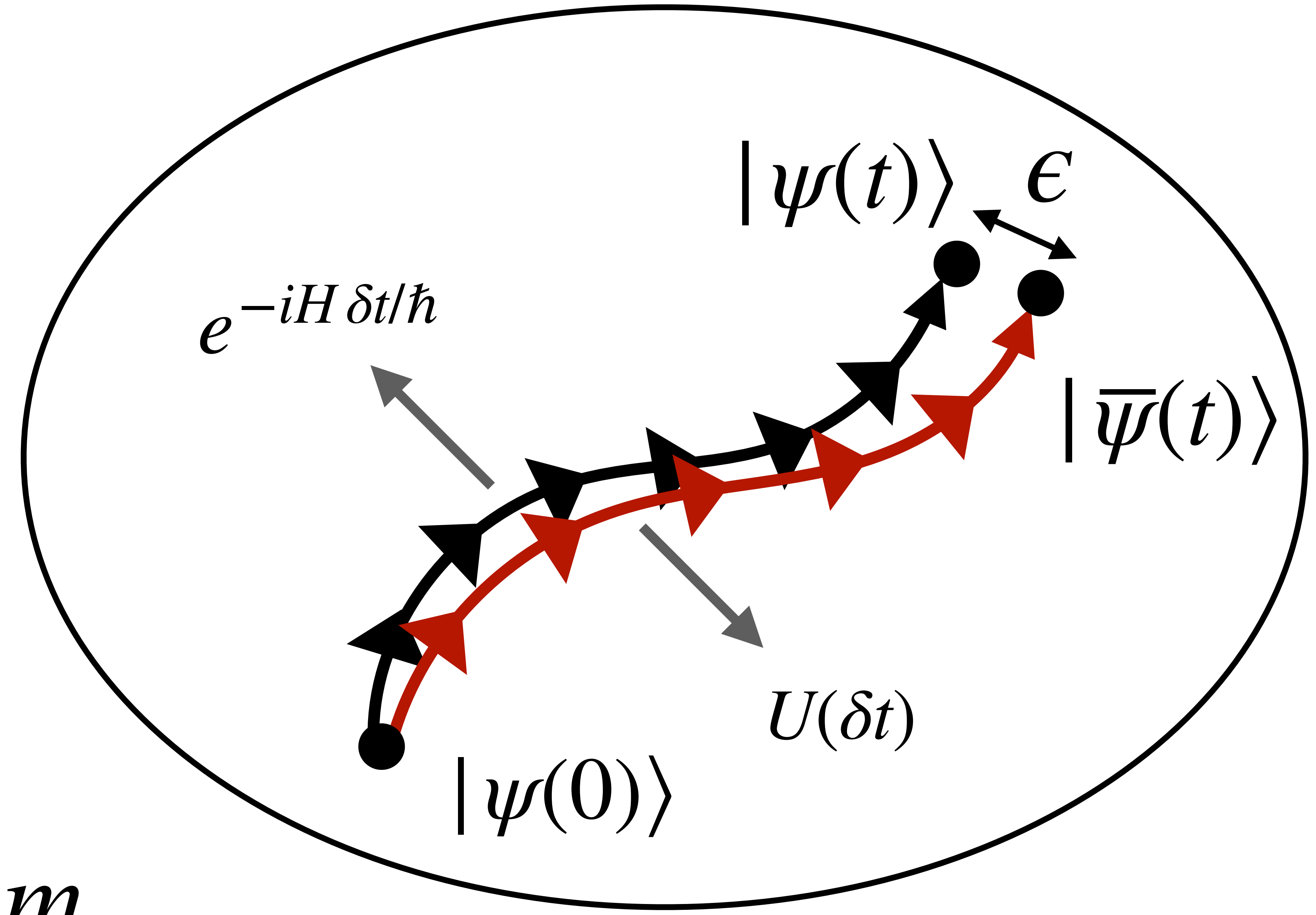
Trotter steps

Trotter time

Trotter, Proc. Amer. Math. Soc. 10 (1959), 545; Suzuki, Commun.Math. Phys. 51, 183 (1976)

Time Evolution in Quantum Computers: Trotterization





$$\delta t = t/m$$

First-order Trotterization

$$U^{(1)}(\delta t) = e^{-iH_1\delta t/\hbar}e^{-iH_2\delta t/\hbar}\ldots e^{-iH_L\delta t/\hbar}$$

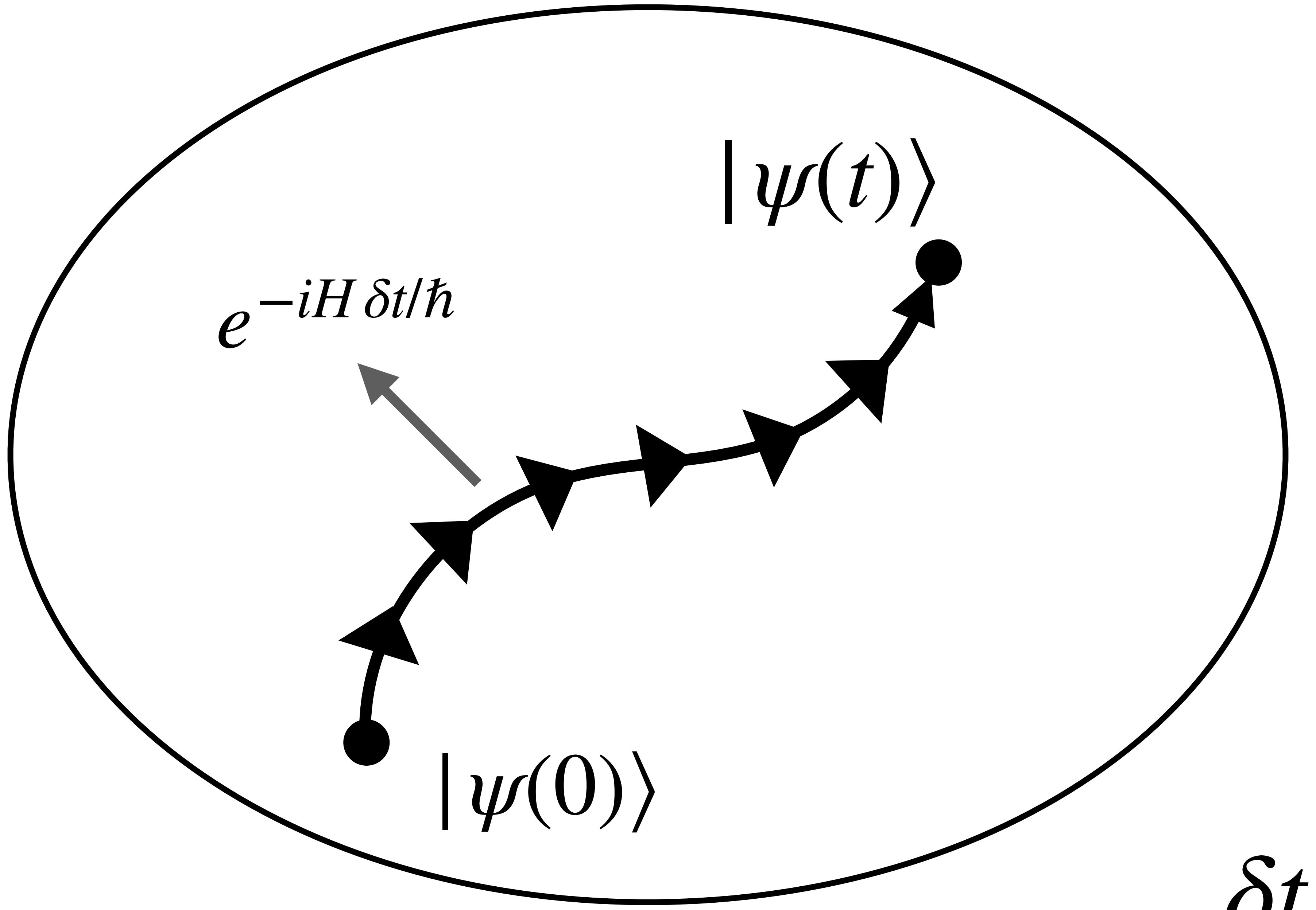
$$\boxed{U^{(k)}(t) = \prod_m U^{(k)}(\delta t)}$$

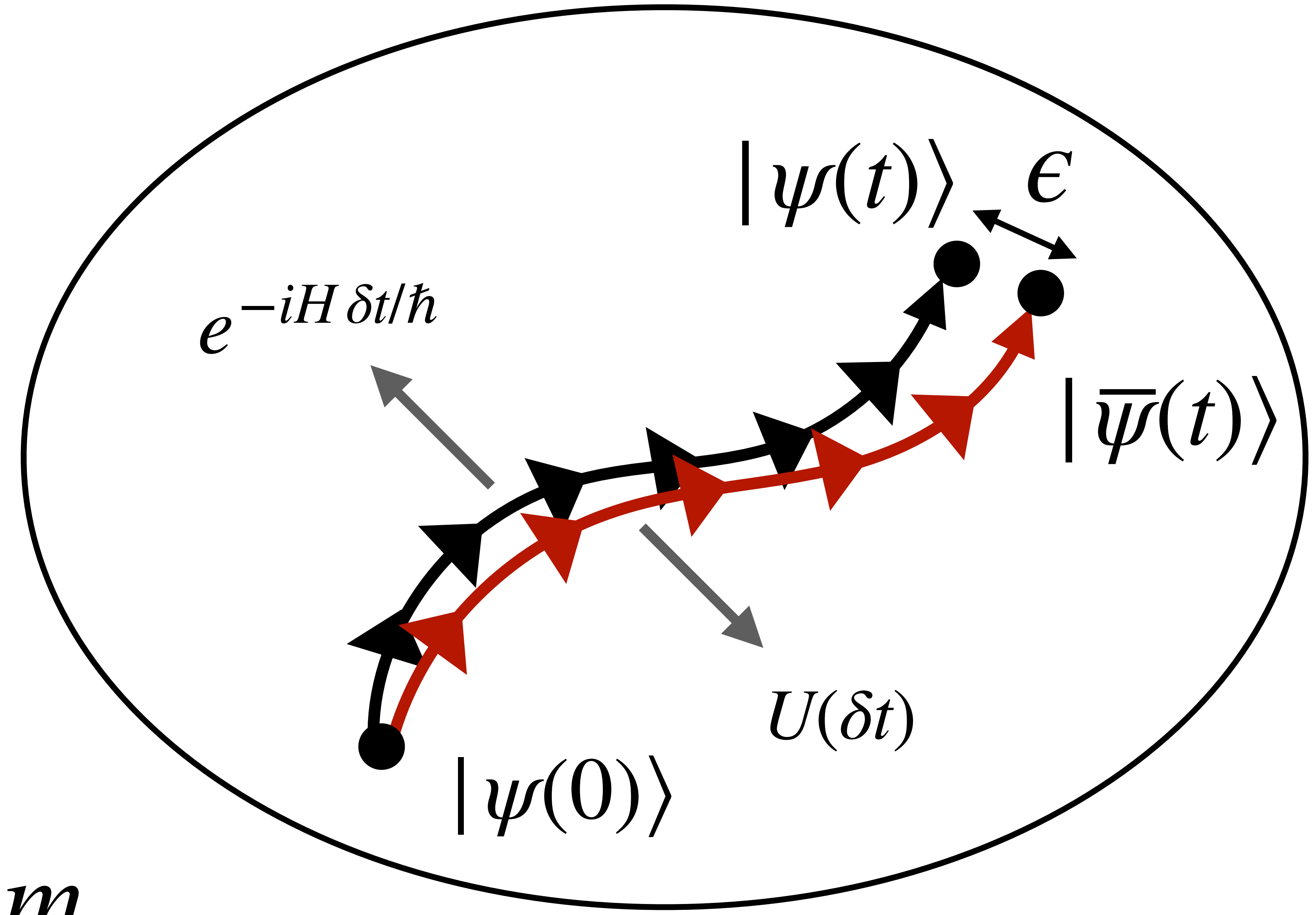
Second-order Trotterization

$$U^{(2)}(\delta t) = \left(e^{-iH_1\delta t/2\hbar}e^{-iH_2\delta t/2\hbar}\ldots e^{-iH_L\delta t/2\hbar}\right)\left(e^{-iH_L\delta t/2\hbar}e^{-iH_{L-1}\delta t/2\hbar}\ldots e^{-iH_1\delta t/2\hbar}\right)$$

Trotter, Proc. Amer. Math. Soc. 10 (1959), 545;
Suzuki, Commun.Math. Phys. 51, 183 (1976)

Time Evolution in Quantum Computers: Trotterization





$$\delta t = t/m$$

First-order Trotter error

$$\epsilon^{(1)} \sim t^2/m$$

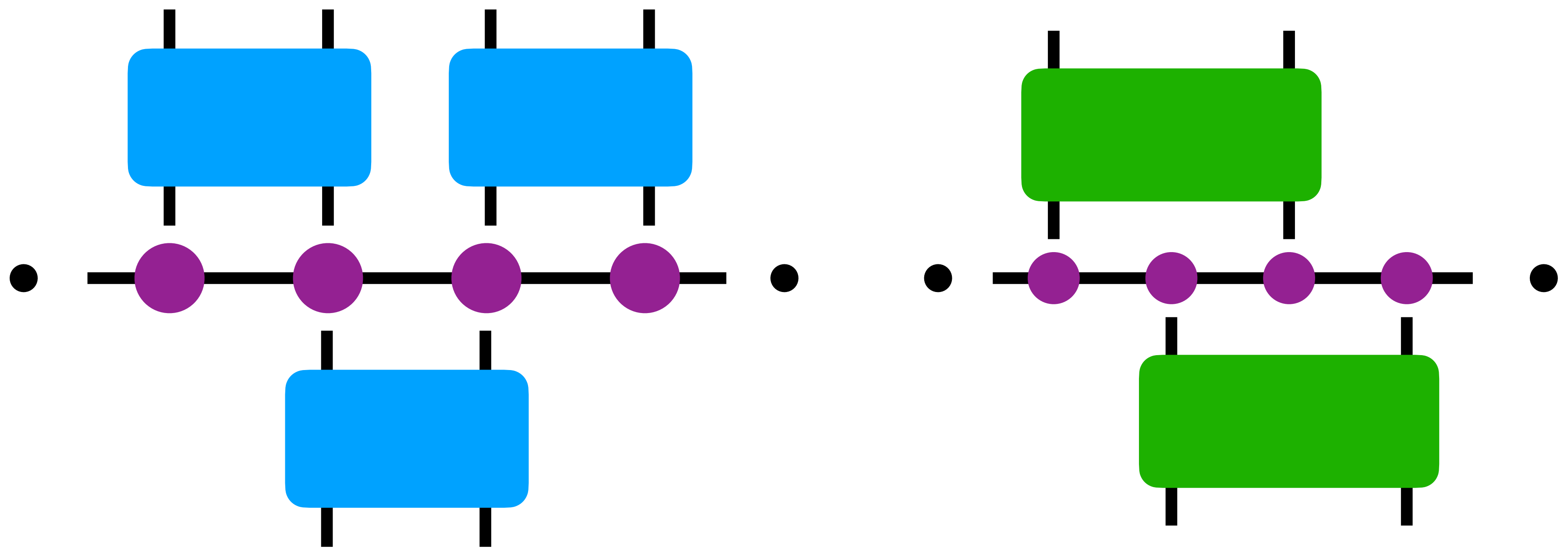
$$U^{(k)}(t) = \prod_m U^{(k)}(\delta t)$$

Second-order Trotter error

$$\epsilon^{(2)} \sim t^2/m^2$$

But leads to larger circuit depth

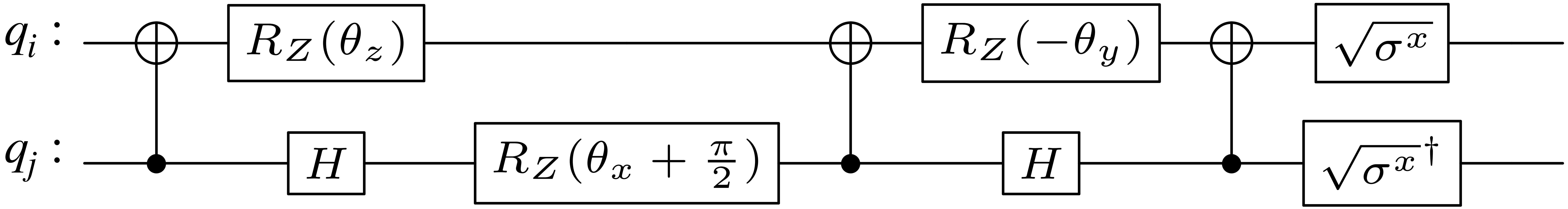
Implementing Trotterization on Quantum Computer



Two-qubit Unitary gate

$$U(\vec{\theta}) = \exp\left[-\frac{i}{2}\left(\theta_x X_i X_j + \theta_y Y_i Y_j + \theta_z Z_i Z_j\right)\right]$$

$U(\vec{\theta}) =$



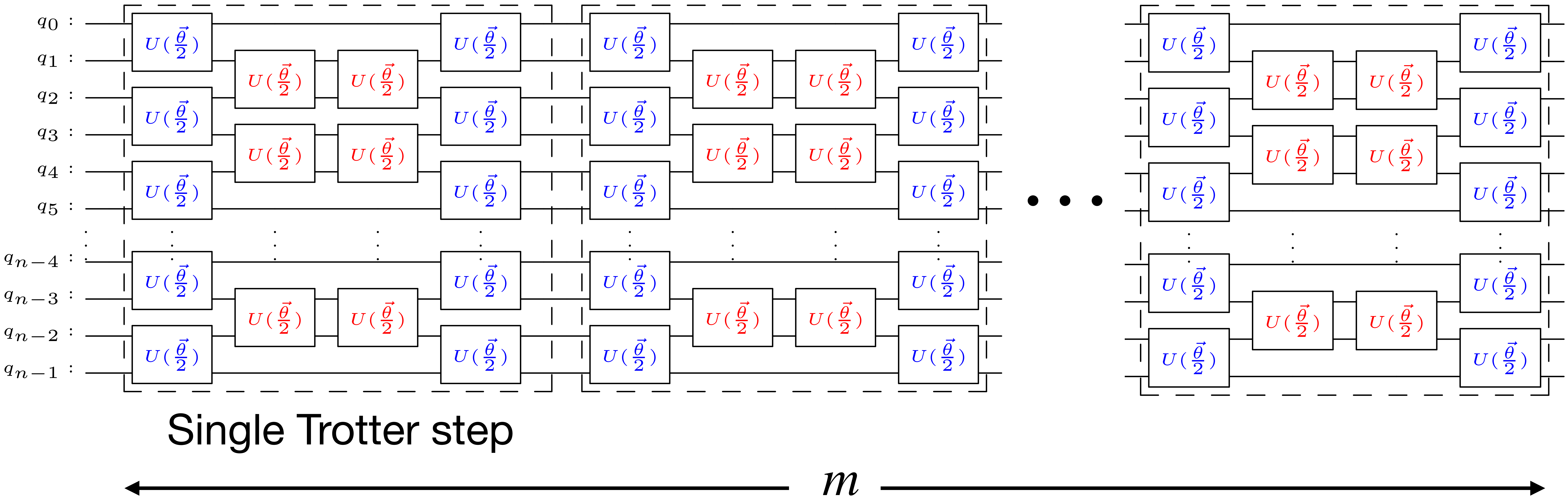
For Isotropic Heisenberg Hamiltonian H_{iso} $\quad \theta_x = \theta_y = \theta_z = 2J_1\delta t \equiv \theta$

For Dimer Hamiltonian H_{Dimer} $\quad \theta'_x = \theta'_y = \theta'_z = J_1\delta t \equiv \theta'$

Zhang et al. arXiv: 2307.16781

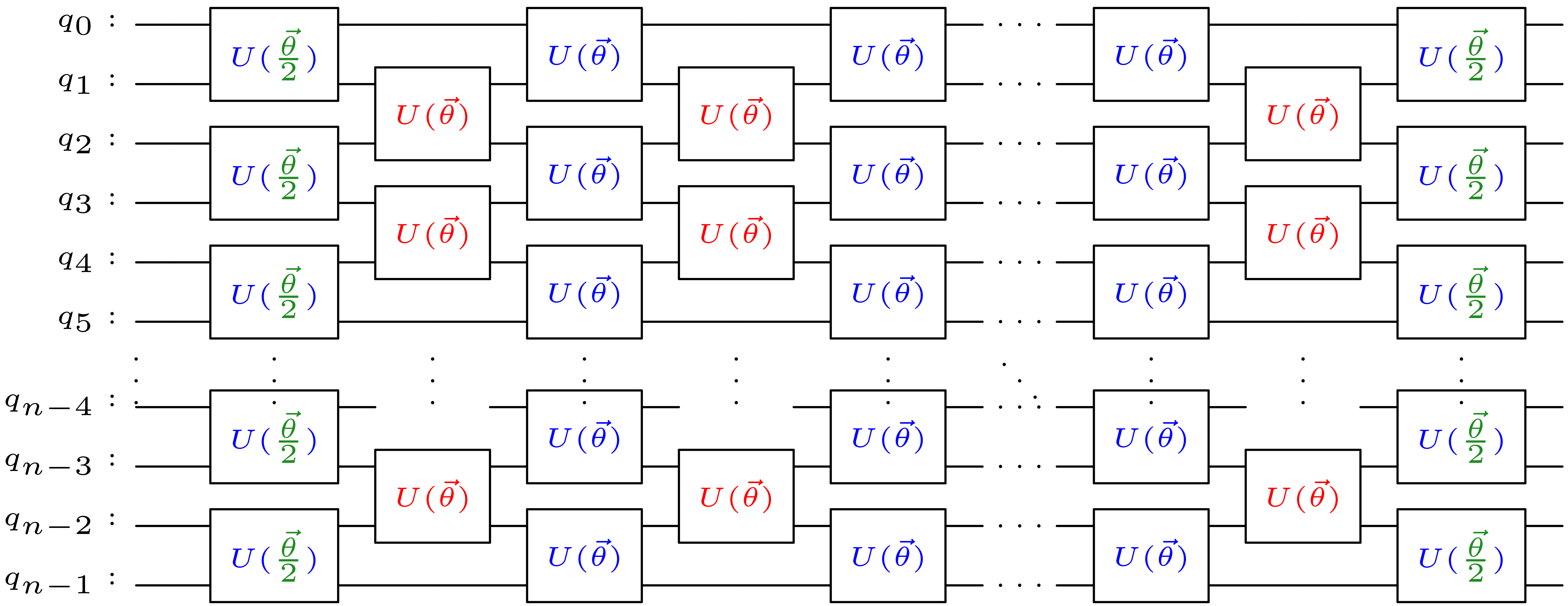
Implementing Trotterization

We implement second-order Trotterization for Isotropic Heisenberg Hamiltonian



Implementing Trotterization

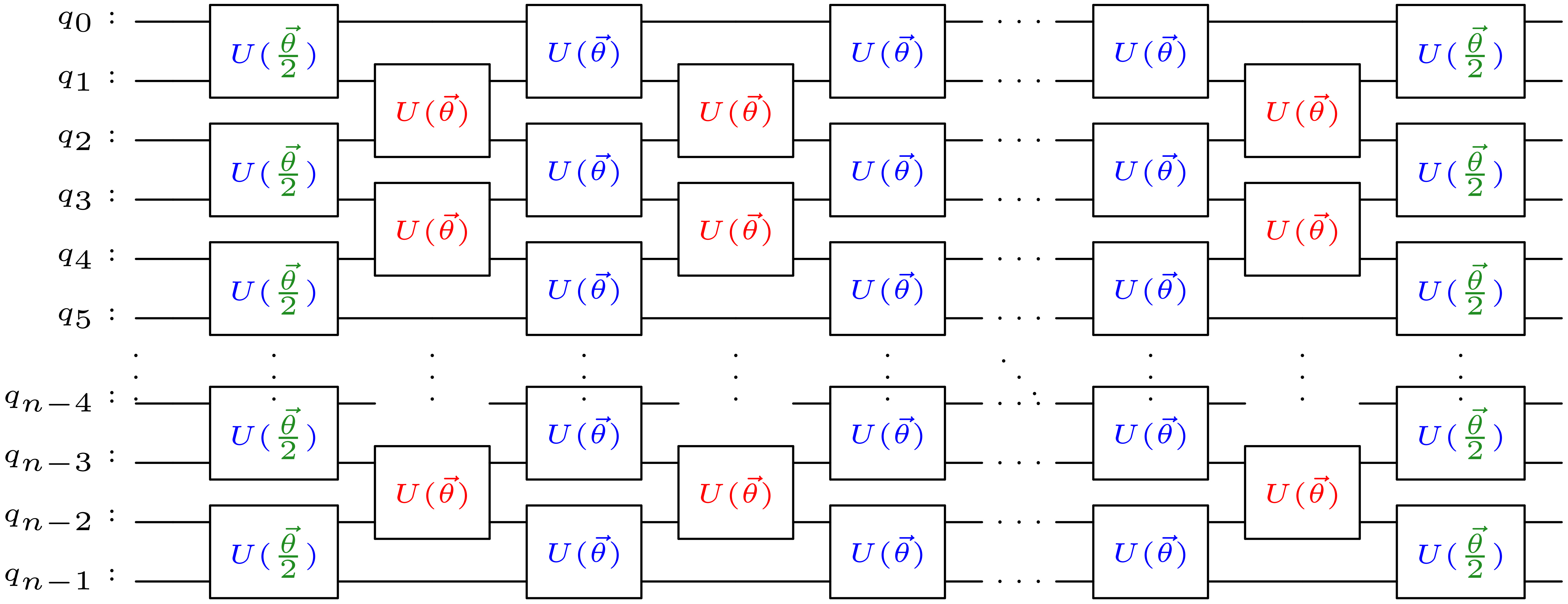
We have optimized second-order Trotterization for Isotropic Heisenberg Hamiltonian

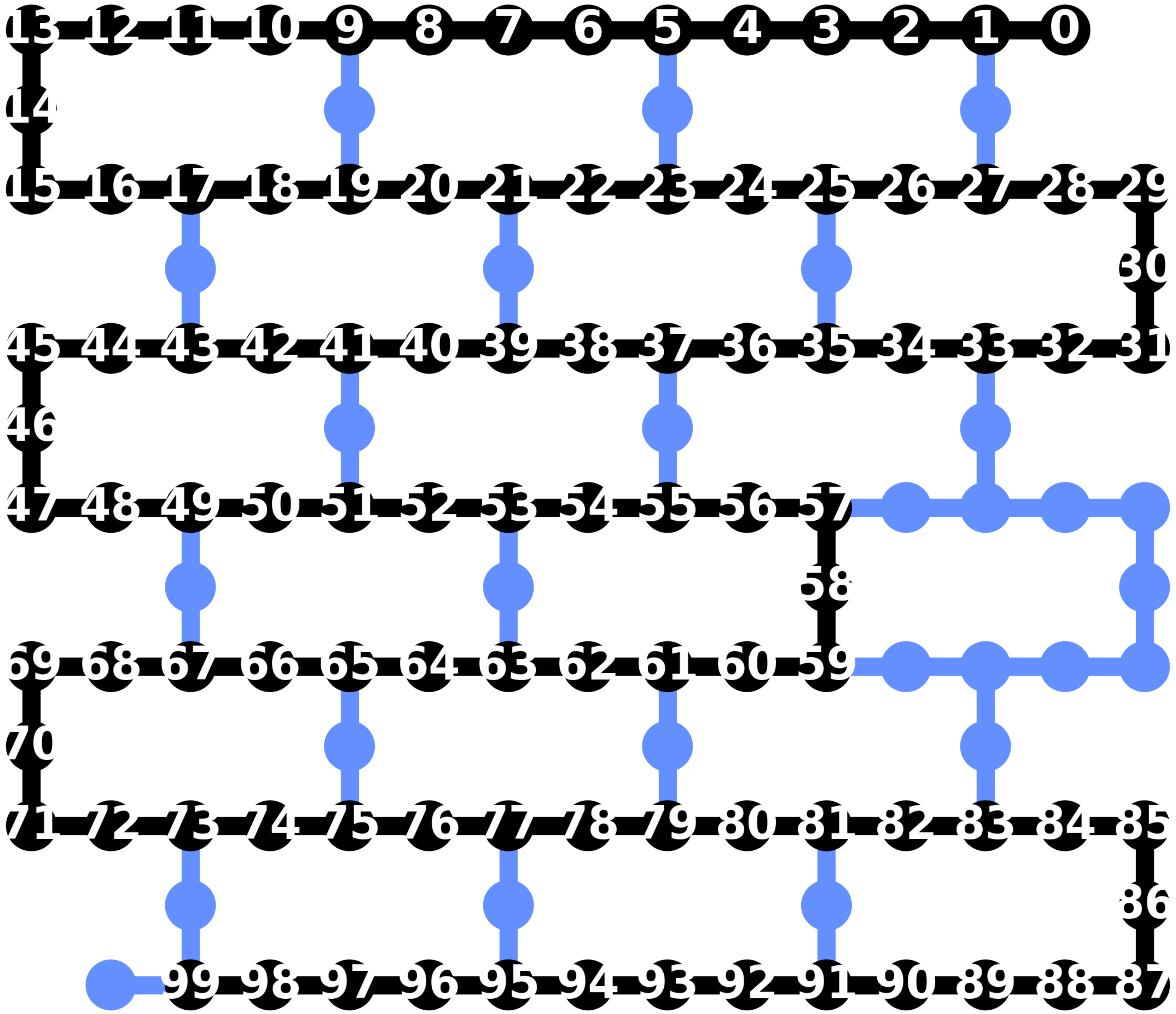


Circuit depth is close to the first-order Trotterization circuit

Implementing Trotterization for Isotropic Hamiltonian H_{iso}

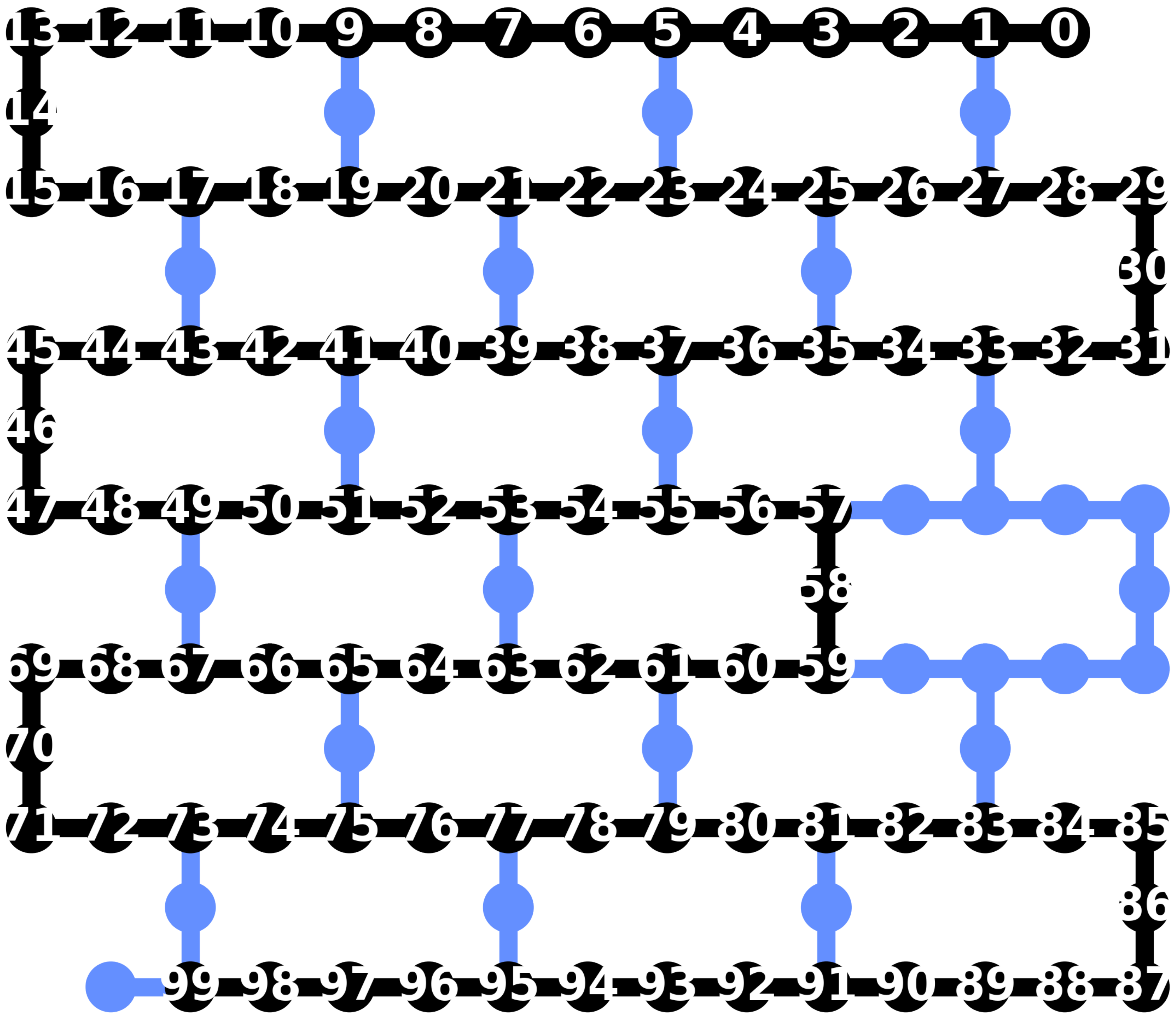
Qubit mapping of $N = 100$ qubits for Isotropic Heisenberg Hamiltonian





ibm_brisbane

Implementing Trotterization for Dimer Hamiltonian H_{Dimer}



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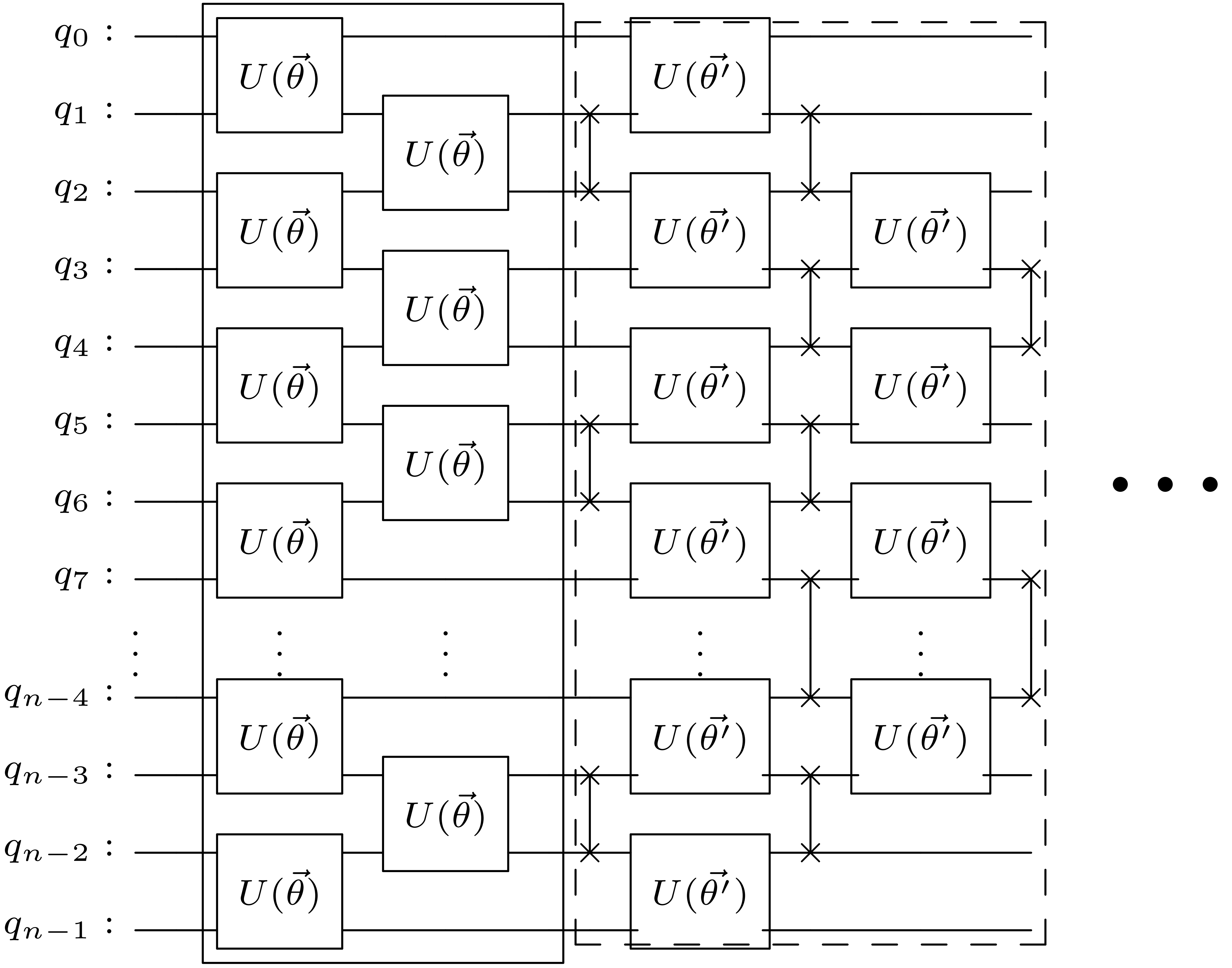


Single Trotter step

Quantum Error Mitigation (QEM)

- Quantum computers are prone to errors.

- Current quantum computers are incapable of correcting errors.

- To utilize today's noisy quantum computers, quantum error mitigation techniques have been developed.

- We applied the following QEM to obtain our expectation value:

  - Zero-noise extrapolation

  - Pauli Twirling

  - Dynamical Decoupling

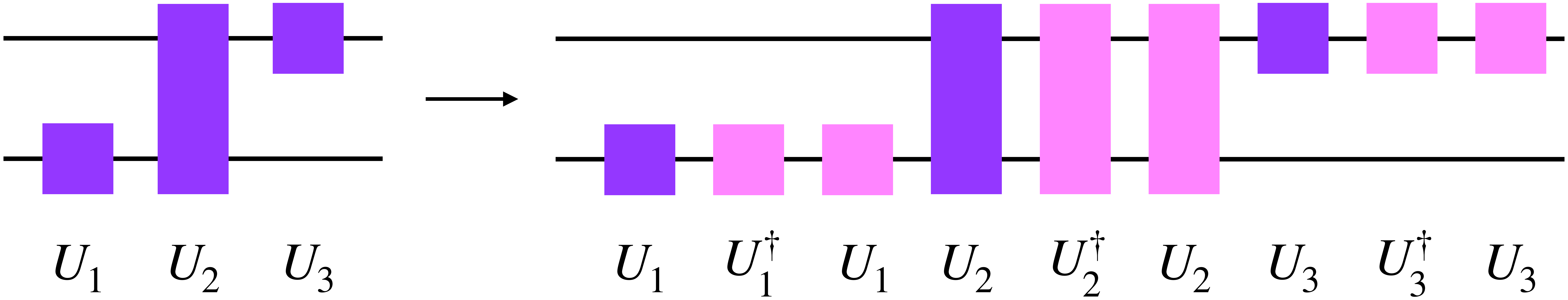
  - Matrix-free Measurement Error Mitigation

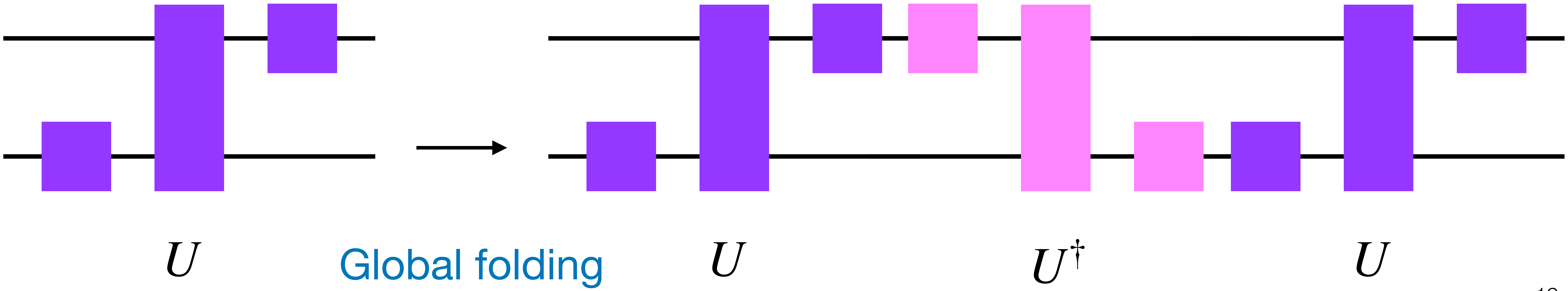
Temme et al., Phys. Rev. Lett. 119, 180509 (2017);
Li et al., arXiv: 1611.09301;
Kandala et al., Nature 567, 491 (2019);
Kim et al., Nature Phys. 19, 752 (2023)

Zero-Noise Extrapolation (ZNE)

- Extracting the expectation value as if the quantum device is noiseless.
- Multiple copies of quantum circuits using Unitary Folding method.

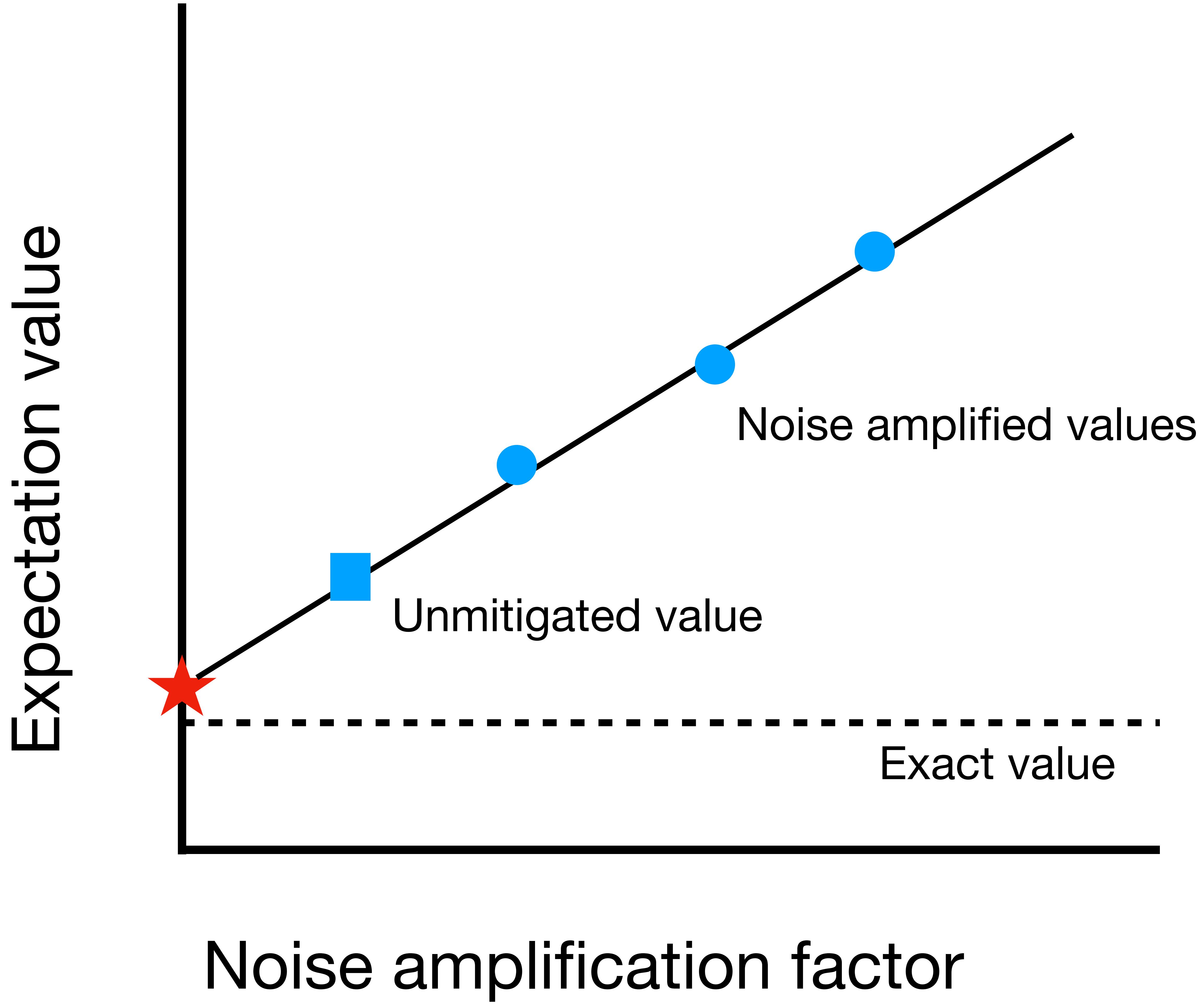
Local folding





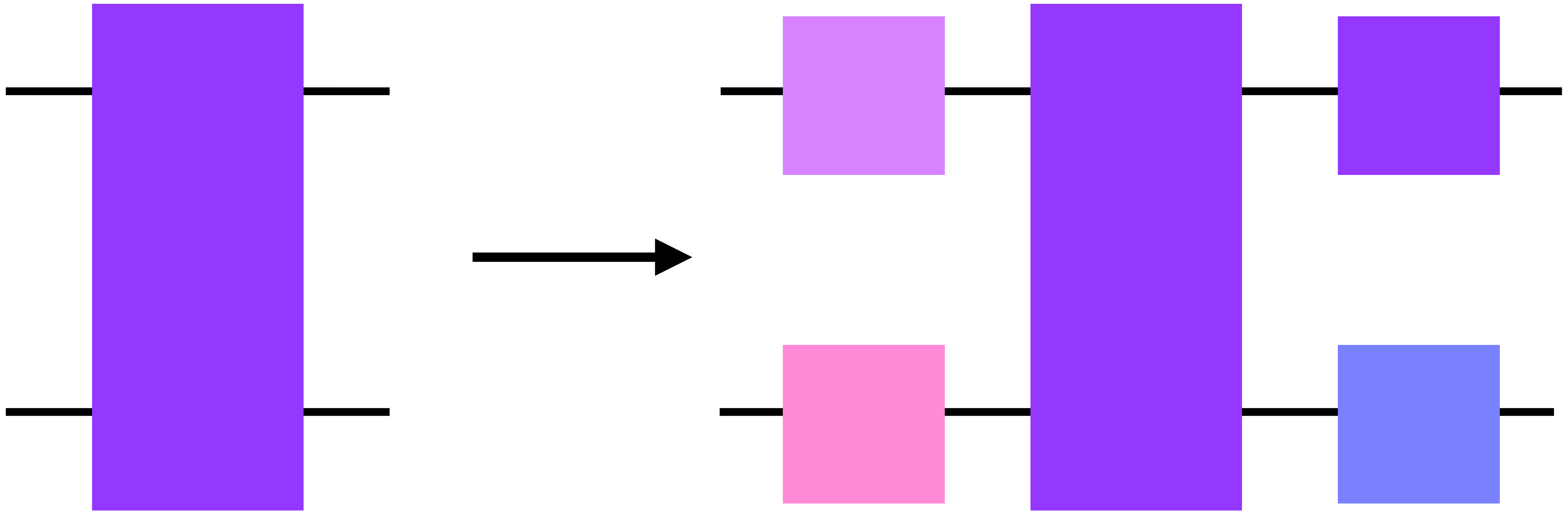
Zero-Noise Extrapolation (ZNE)

- Extracting the expectation value as if the quantum device is noiseless
- Multiple copies of quantum circuits using Unitary Folding method.



Pauli Twirling

- Pauli twirling is a method averaging out the off-diagonal coherent errors of the circuits in the Pauli basis: {I, X, Y, Z}.

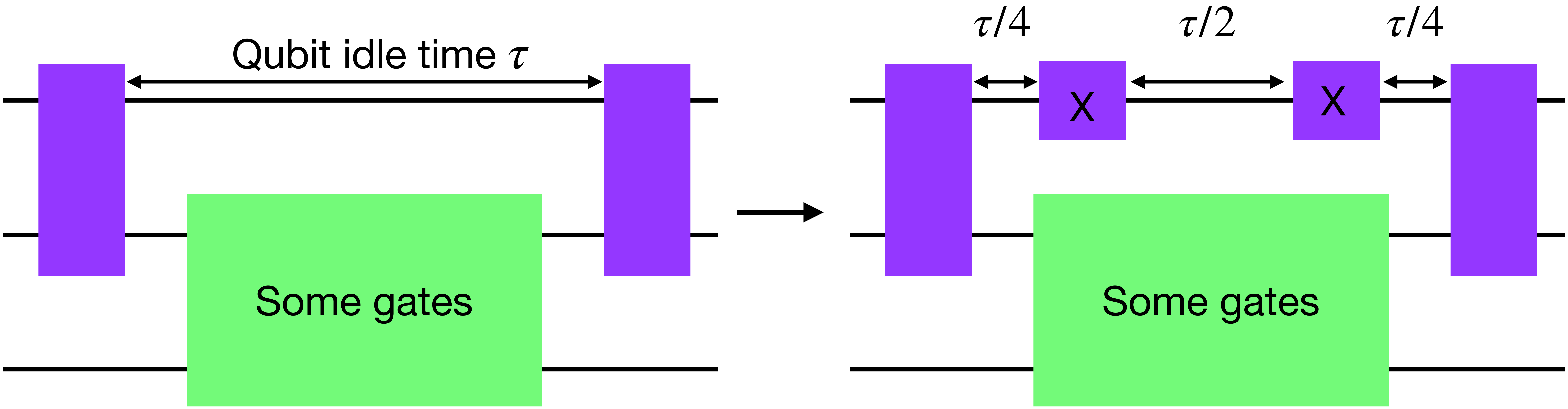


- This process is repeated multiple times, with different random Pauli operators applied each time.

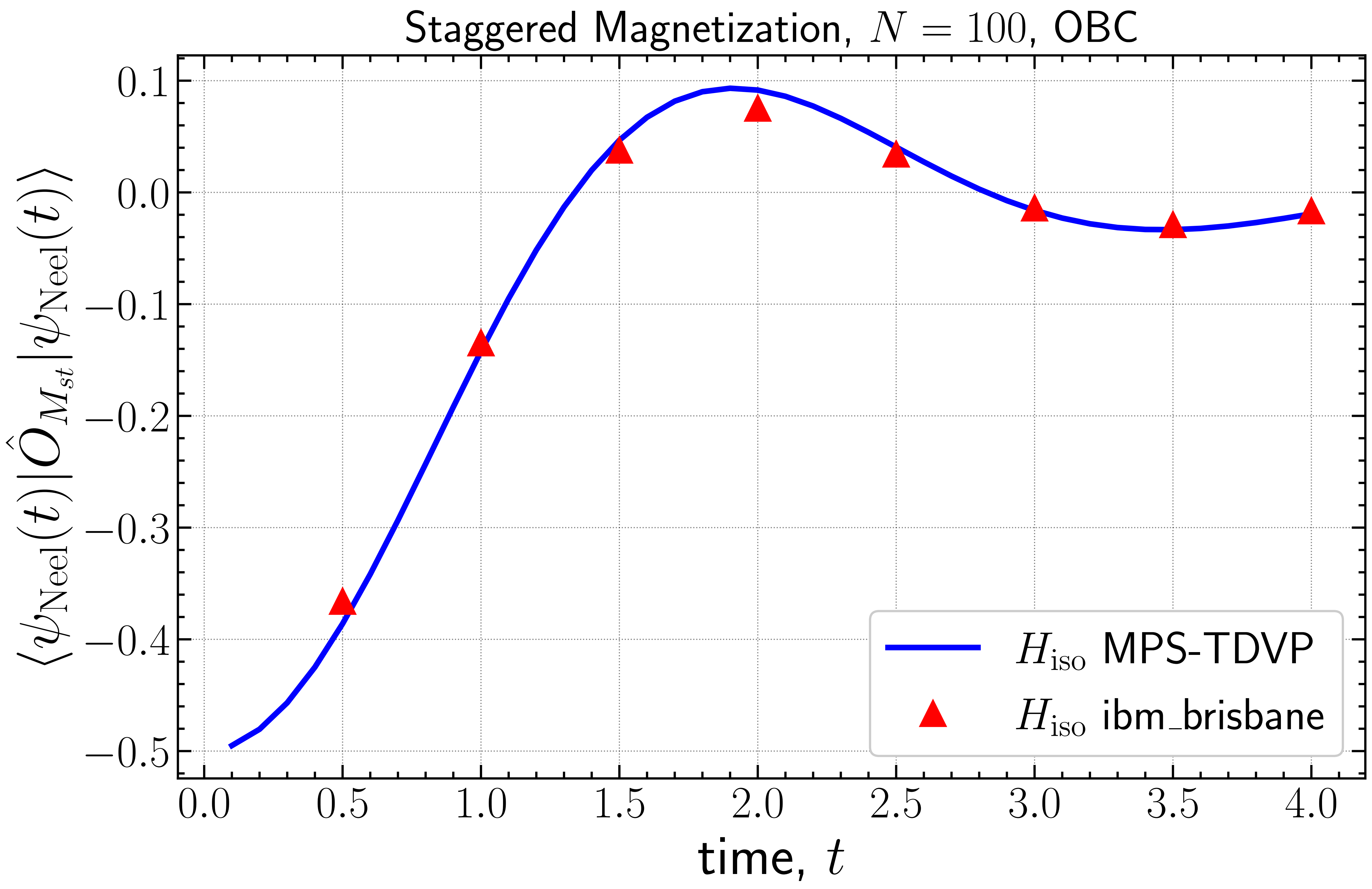
- The results of these many "twirled" circuits are then averaged.

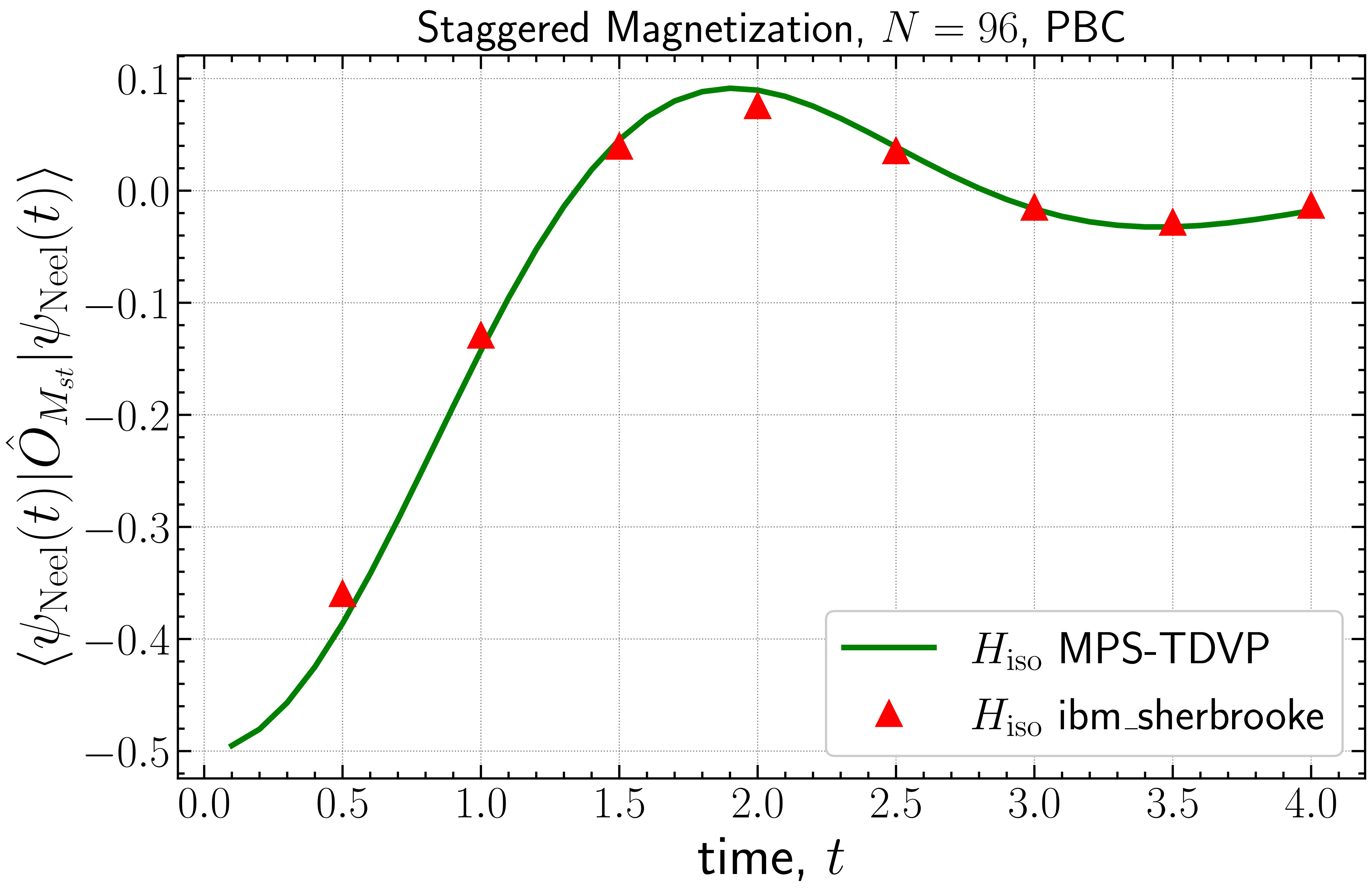
Dynamical Decoupling

- Dynamical Decoupling (DD) is a QEM method which reduces error caused by idle or spectator qubit.



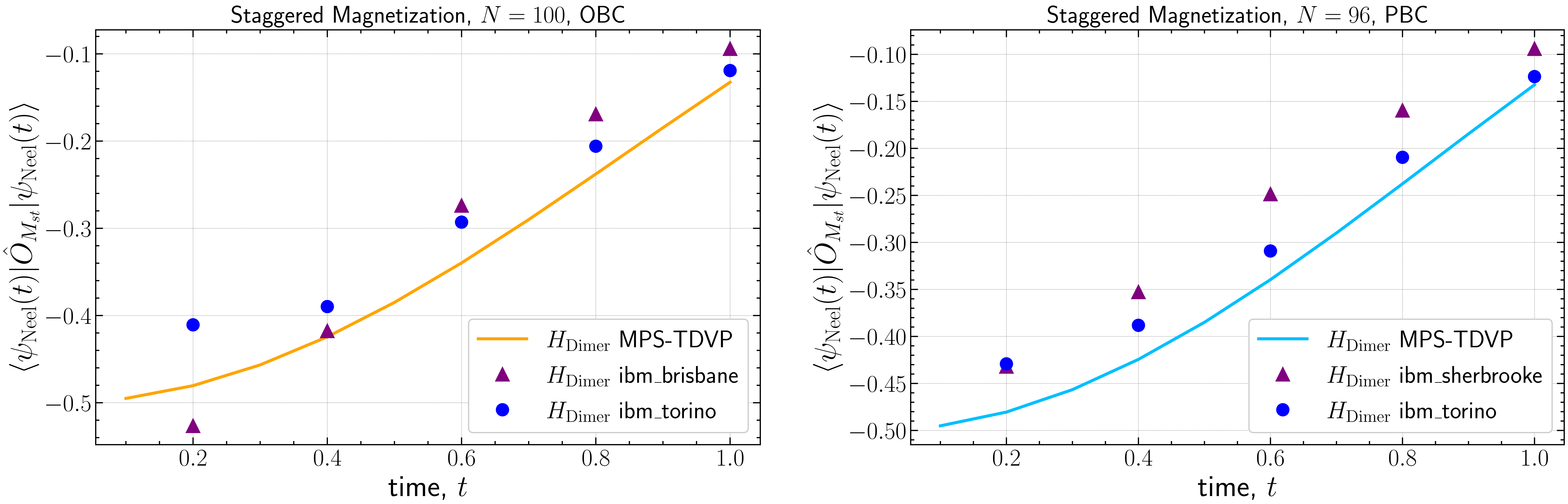
Staggered Magnetization Variation for H_{iso}



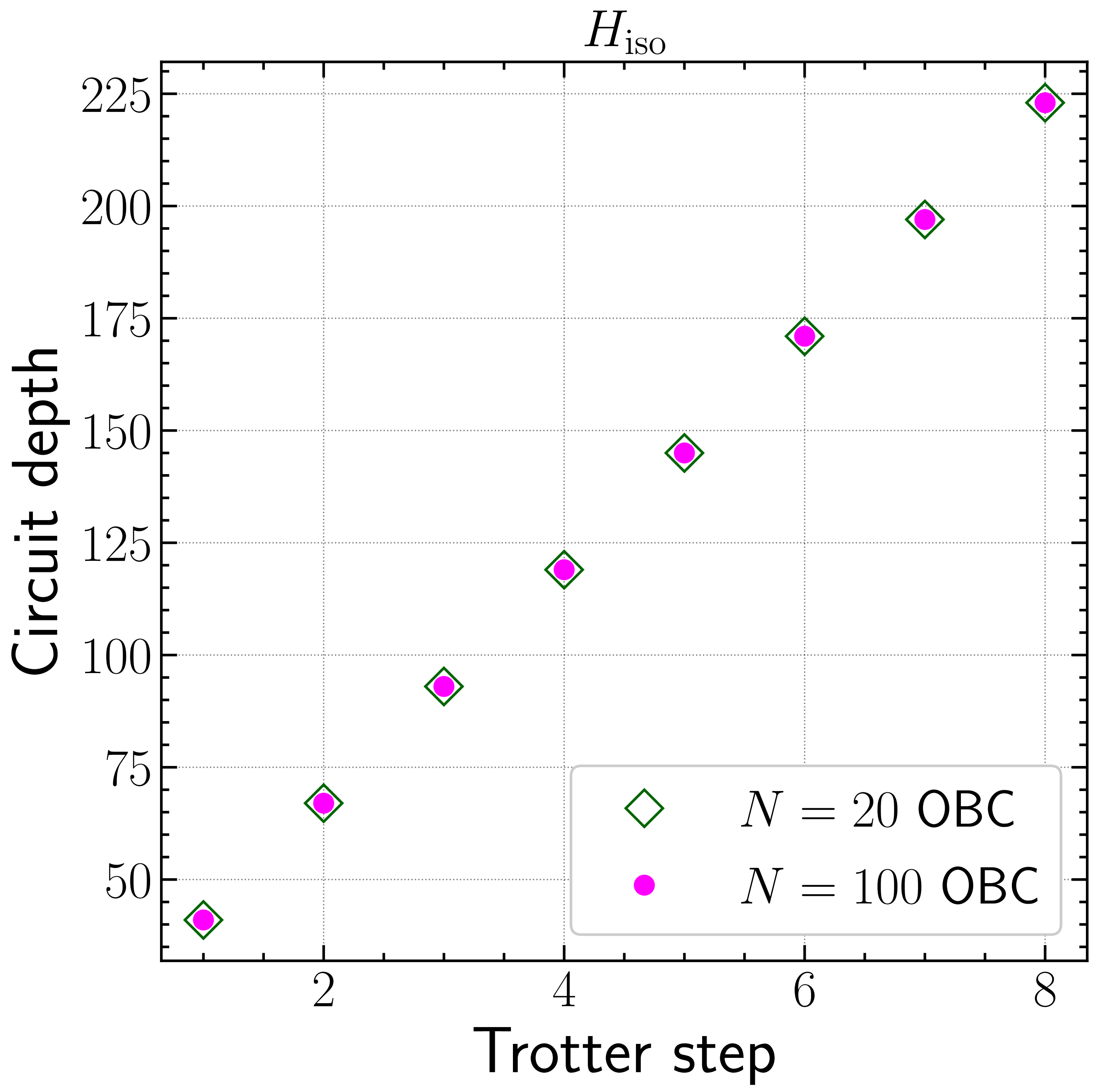


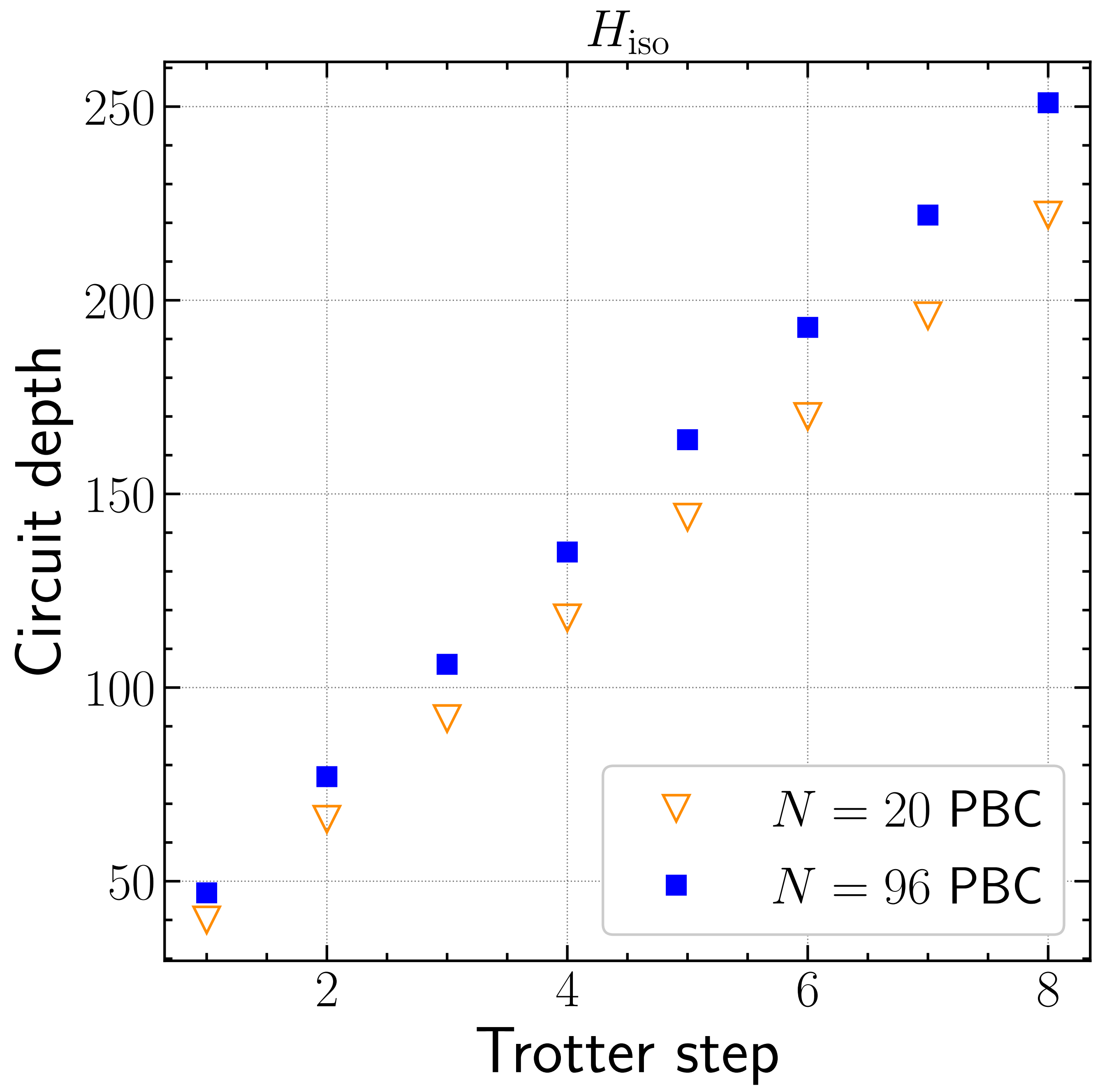
Matrix Product State based
Time dependent Variational Principle (MPS-TDVP):
Haegeman et al., Phys. Rev. Lett. 107, 070601 (2011)

Staggered Magnetization Variation for H_{Dimer}

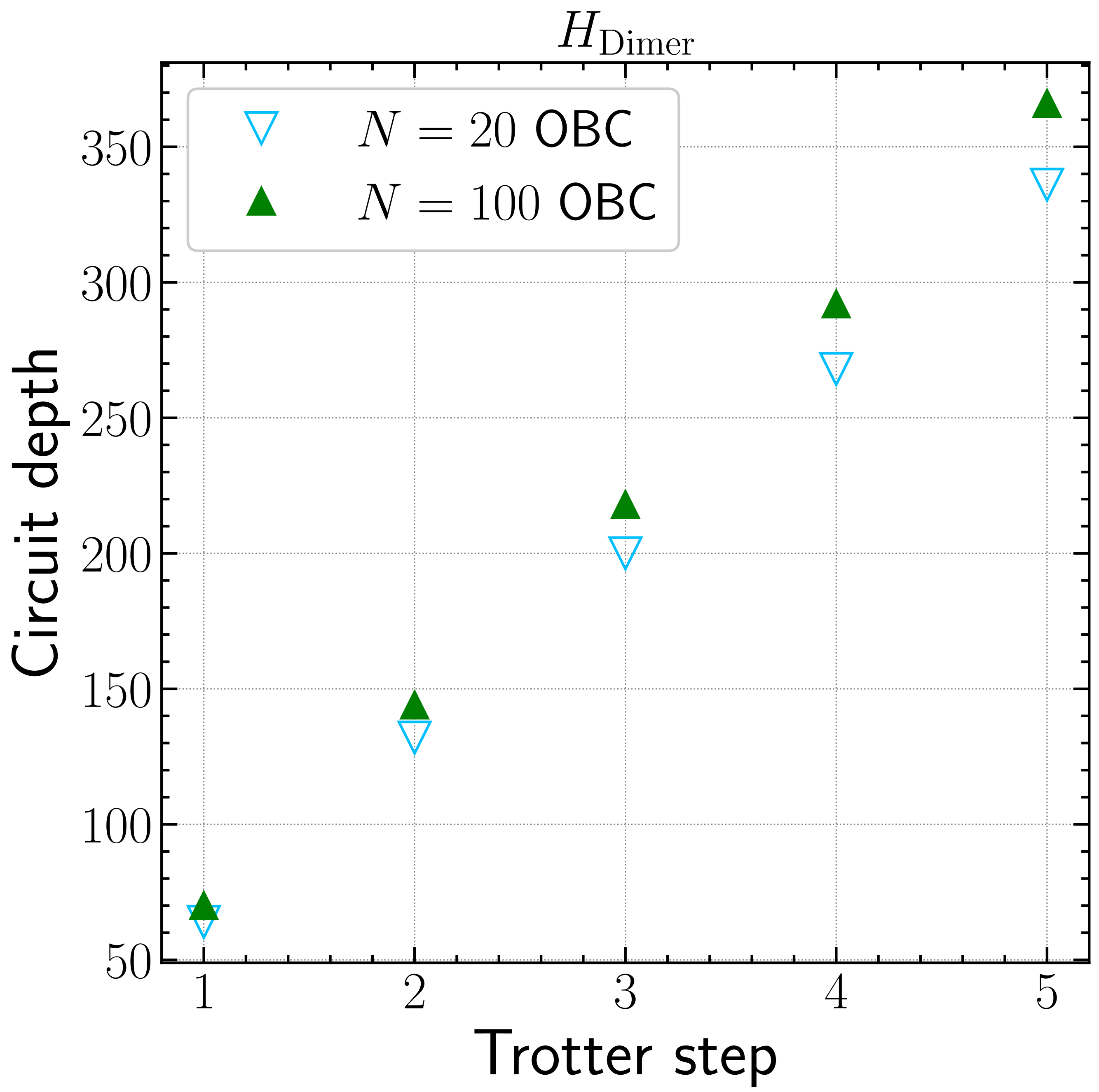


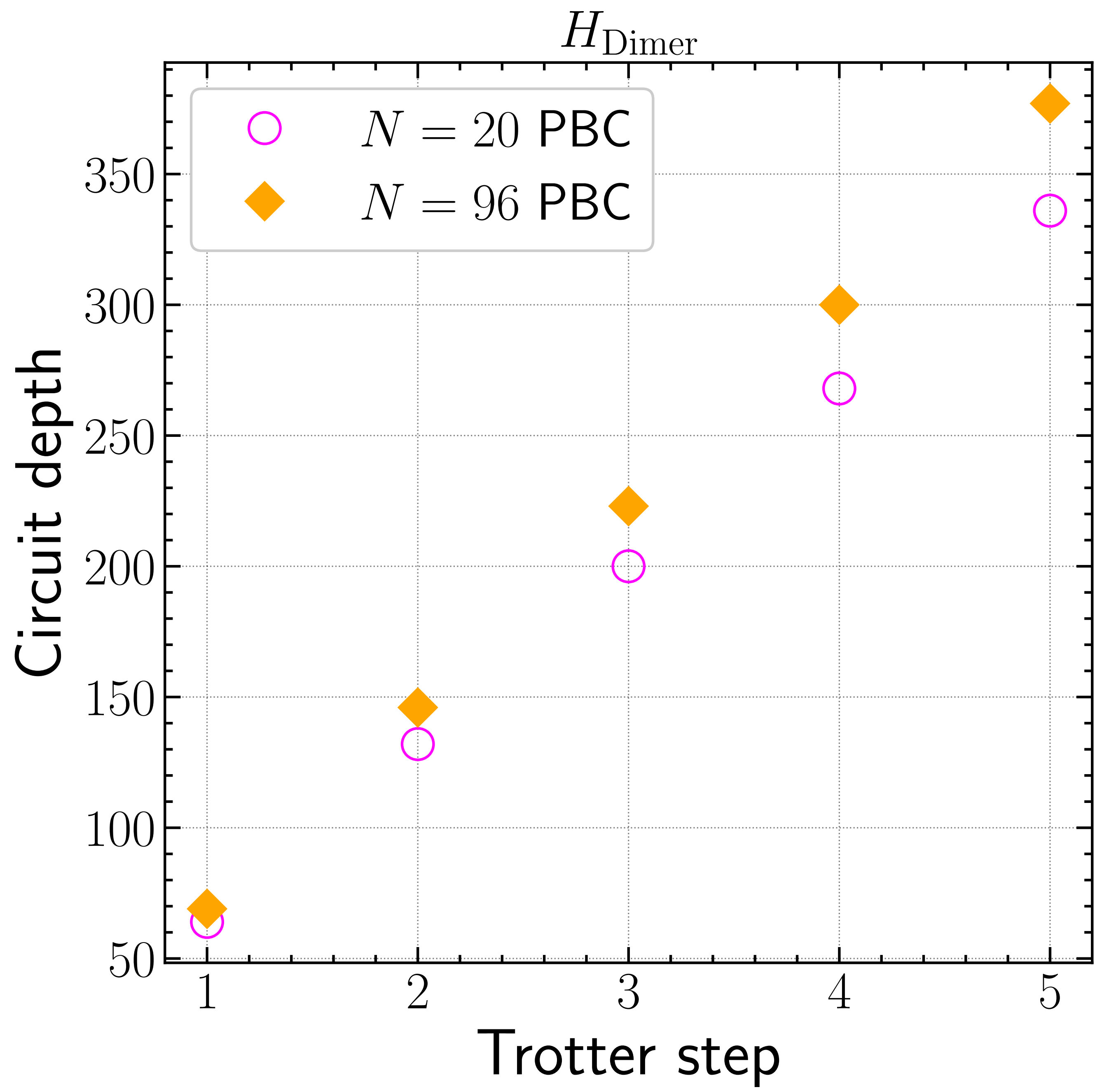
Circuit Depth and Scalable Quantum Circuit





Isotropic Hamiltonian





Dimer Hamiltonian

Conclusion and Outlook

- By combining the Quantum Error Mitigation methods, we achieve better accuracy on noisy IBM quantum hardwares for large-scale spin-chain problem.

- Our optimized Trotterization quantum circuits are scalable.

- Currently for 1D spin chain problem, Tensor network based methods are competitive.

- But Tensor network based methods require exponential computational resource when it comes to highly entangled state at a large scale.

- Time evolution brings a quantum state of low entanglement to a highly entangled state.

- Quantum computer, in coming days, will go beyond such entanglement barrier and explore uncharted complex dynamics of quantum many-body systems.