# Exponential distillation of dominant eigenproperties

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**GPU Day 2025**

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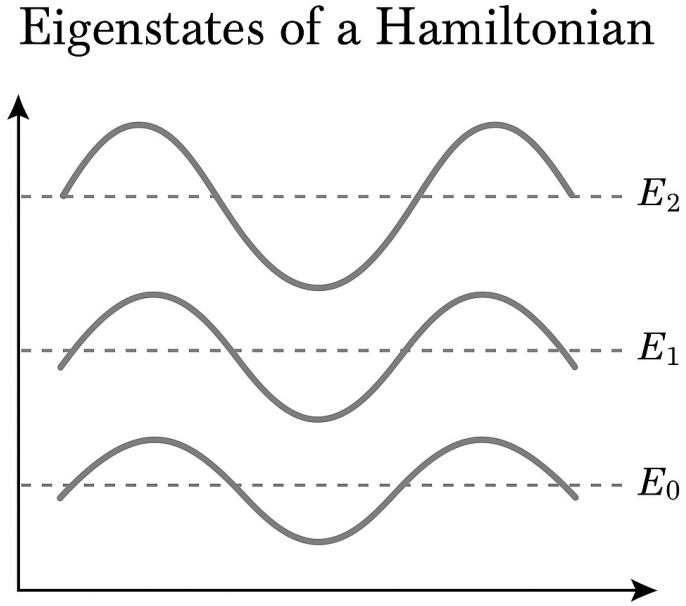
# Outline

1. Problem formulation
2. Existing approaches and their limitations
3. Performance guarantees
4. The DDE algorithm
5. Numerical experiments

# Eigenstate property estimation




**Inputs**:
- Hamiltonian: $\mathcal{H} = \sum_k E_k |\psi_k\rangle\langle\psi_k|$
- Observable: $O$

**Common assumptions**:
- Initial state: $|\psi(0)\rangle = \sum_k c_k |\psi_k\rangle$

  Dominant eigenstate:

  $|\psi_q\rangle$ ($|c_q| > |c_k|$ for all $k \neq q$)

- Nonvanishing gap: $\Delta > 0$

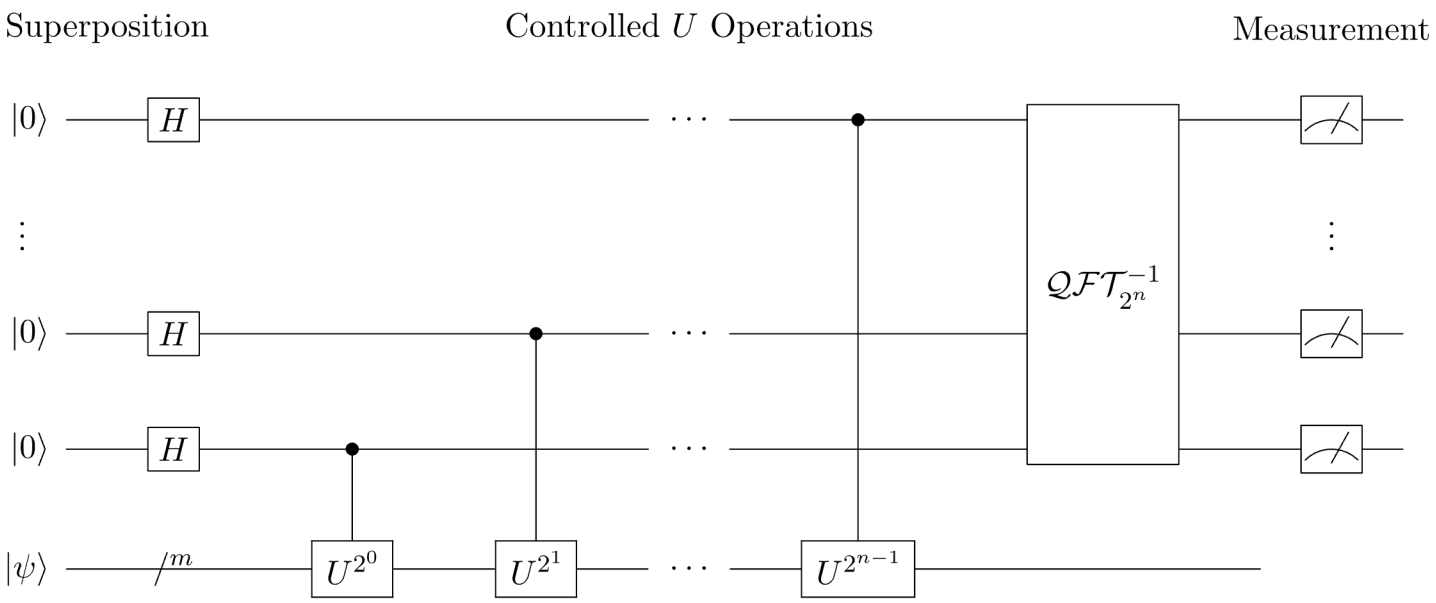
**Goal**:

Estimate $\langle\psi_q|O|\psi_q\rangle$

for target eigenstate $|\psi_q\rangle$

# Fault-tolerant strategies

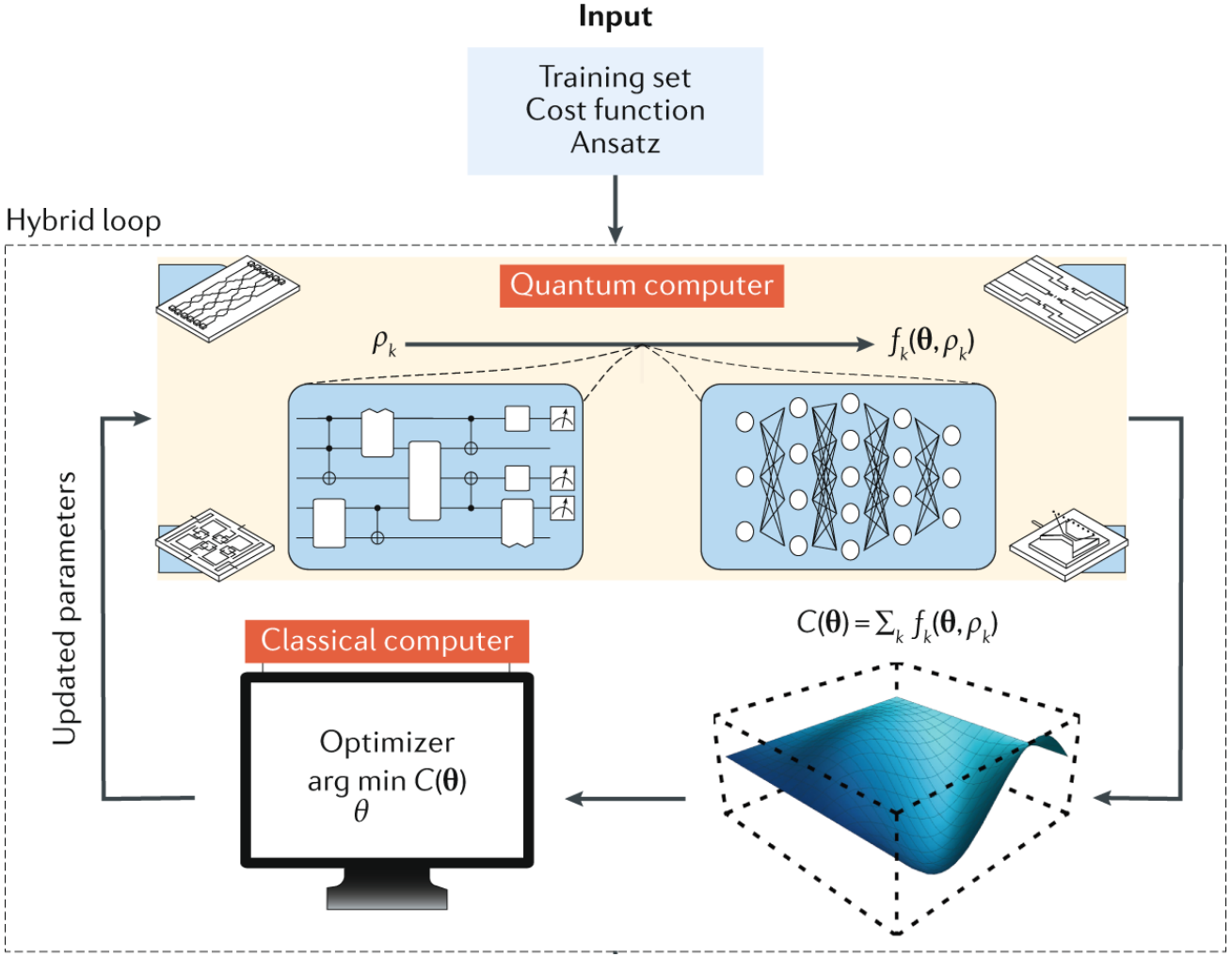
## Quantum Phase Estimation (QPE)




Resource requirements:
- Deep circuits
- Error corrected qubits

A. Y. Kitaev. Quantum Measurements and the Abelian stabilizer problem. arXiv:quant-ph/9511026 (1995)

# Near-term approaches




M. Cerezo et al., Variational quantum algorithms. Nat Rev Phys 3, 625-644 (2021).

## Variational techniques

Limitations:

- No converge guarantees
- Trainability issues

# Dealing with these challenges

Offload some computational burden to a classical computer in post-processing!

Compatible with both types of techniques!

# Lemma 1: Random time evolution

We consider the **average state**:

Pure time eviolved state: $\rho(t) = e^{-it\mathcal{H}}|\psi(0)\rangle\langle\psi(0)|e^{it\mathcal{H}}$

$$\bar{\rho} = \mathbb{E}_t[\rho(t)] = \int_{-\infty}^{\infty} G(t)\,\rho(t)\,\mathrm{d}t = \rho + \mathcal{E}$$

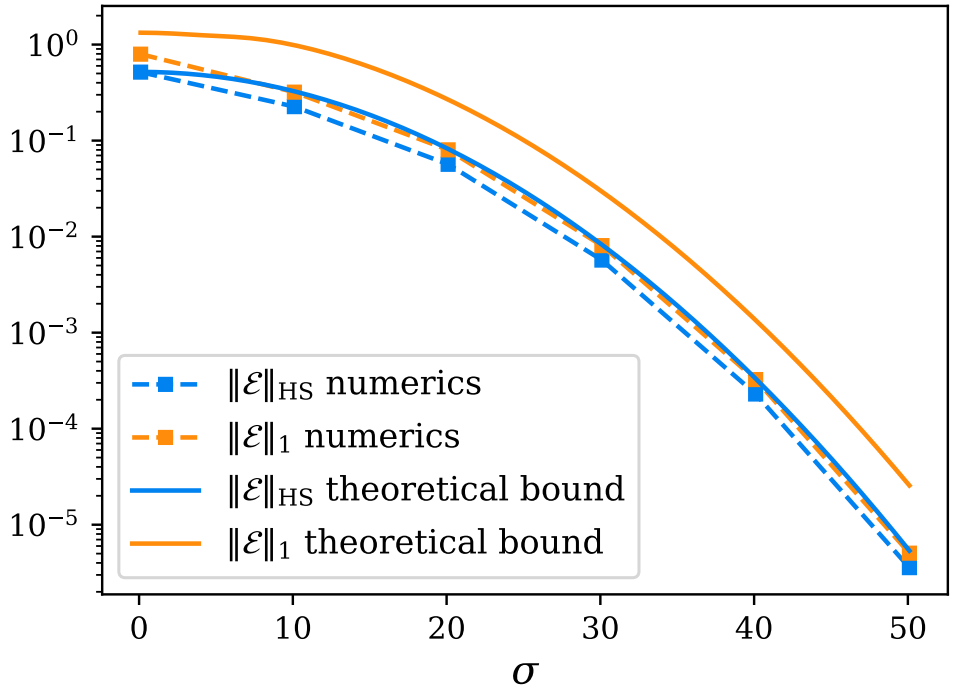
**Error term vanishes** super-exponentially in $\sigma$

**Gaussian PDF** with std. $\sigma$

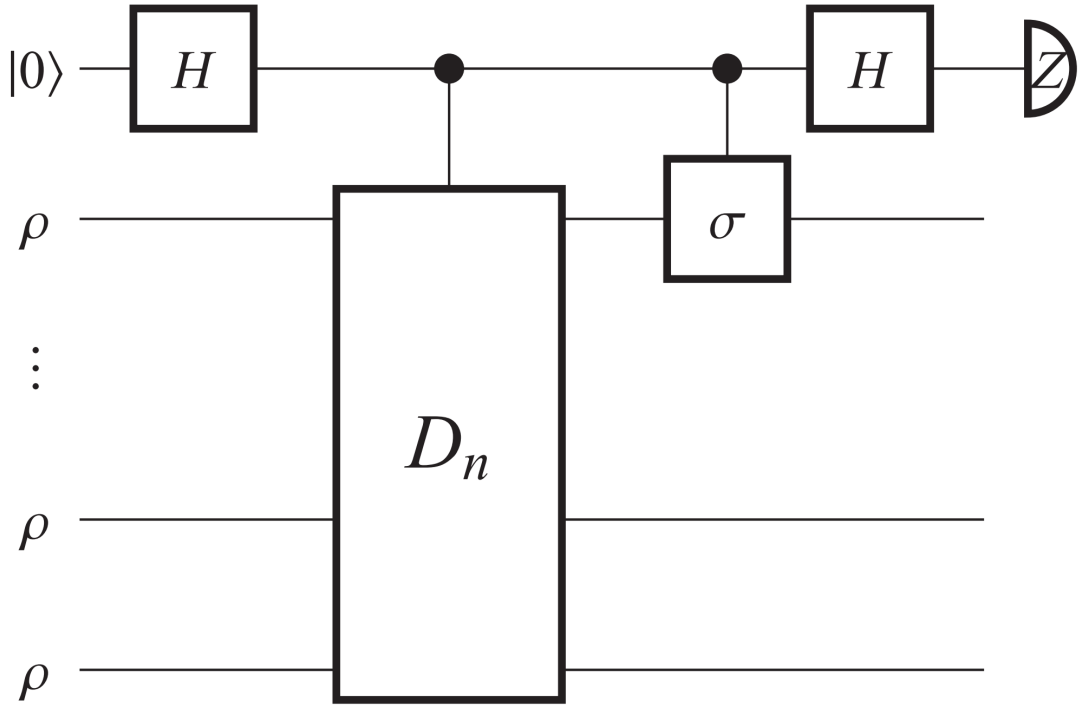
$$G(t) = \left(\sqrt{2\pi}\sigma\right)^{-1} e^{-\frac{t^2}{2\sigma^2}}$$

**Diagonal state**

$$\rho = \sum_k p_k\,|\psi_k\rangle\langle\psi_k|, \text{ where } p_k = |c_k|^2$$



# Lemma 2: Virtual distillation (VD)




Property of interest

$$\frac{\mathrm{Tr}[\rho^n O]}{\mathrm{Tr}[\rho^n]} = \langle\psi_q|O|\psi_q\rangle + \mathcal{A}$$

Nonlinear functionals

**Error term vanishes**
exponentially in $n$

B. Koczor, Exponential error suppression for near-term quantum devices, Phys. Rev. X 11, 031057 (2021).

# Theorem 1: Applying VD

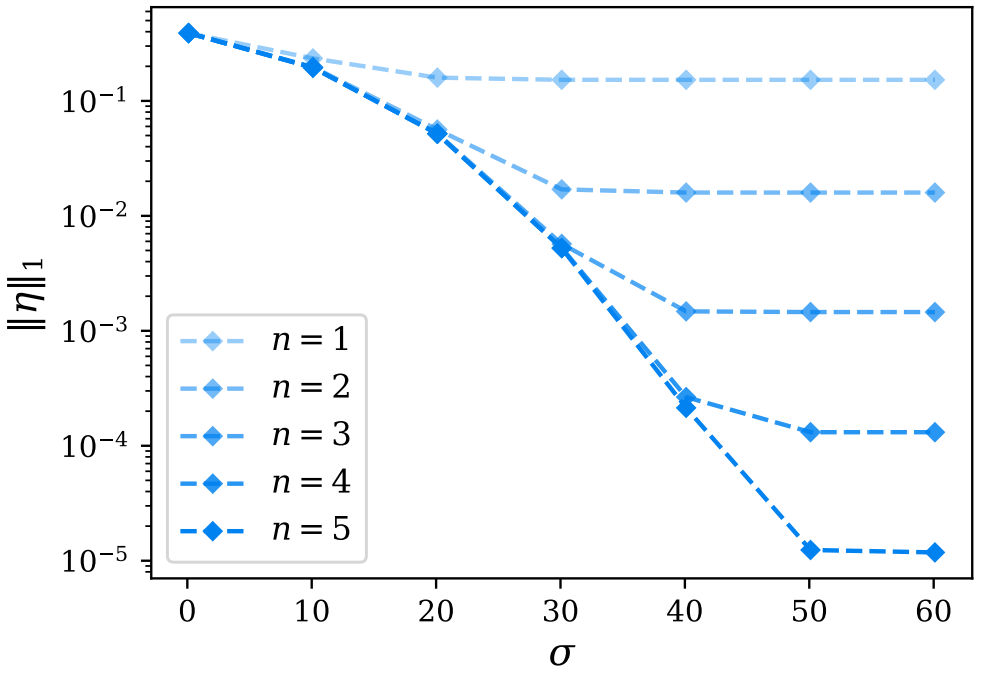
Nonlinear functionals of average state

$$\frac{\mathrm{Tr}[\bar{\rho}^n O]}{\mathrm{Tr}[\bar{\rho}^n]} = \langle \psi_q | O | \psi_q \rangle + \mathcal{Q}$$

$$|\mathcal{Q}| \leq |\mathcal{A}| + 4np_q^{-1}||O||_\infty ||\mathcal{E}||_1 + \mathcal{O}(||\mathcal{E}||_1^2)$$

Vanishes super-exponentially with σ

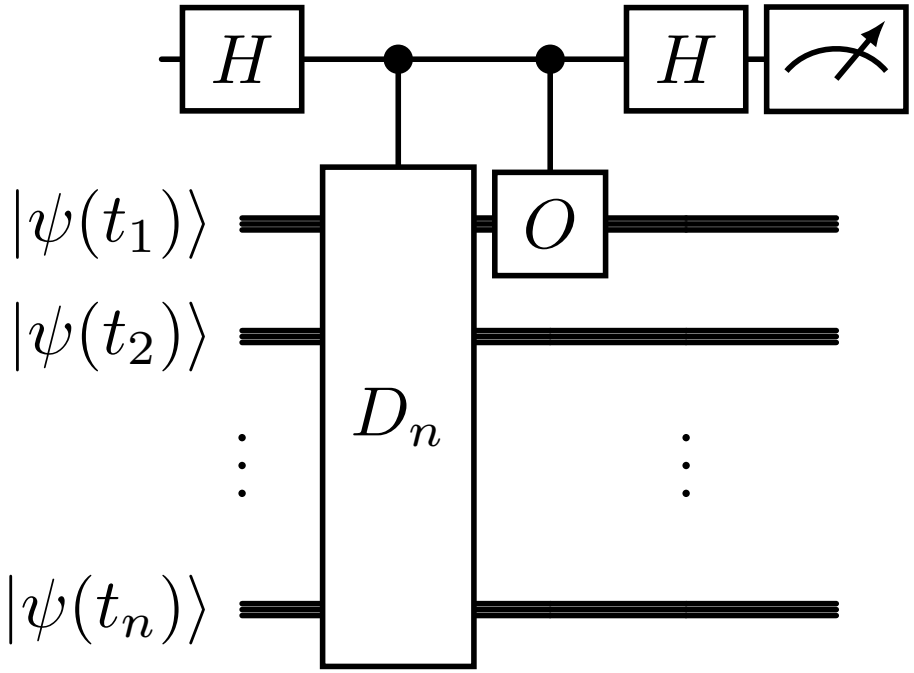
Vanishes exponentially with $n$




$$\eta = \bar{\rho}^n / \mathrm{Tr}[\bar{\rho}^n] - |\psi_q\rangle\langle\psi_q|$$

# Direct implementation

1. Sample time values $\boldsymbol{t} = (t_1, \ldots, t_n)$
2. Run Hadamard test circuit
3. Repeat multiple times



# Distillation of dominant eigenproperties (DDE)

$$\frac{\mathrm{Tr}[\bar{\rho}^n O]}{\mathrm{Tr}[\bar{\rho}^n]} = \langle \psi_q | O | \psi_q \rangle + \mathcal{Q}$$

**Evaluate these nonlinear functionals through Monte Carlo (MC) integration!**

MC 1

$$\mathrm{Tr}[\bar{\rho}^n O] = \int G(\boldsymbol{t}) F(\boldsymbol{t}) \mathrm{d}\boldsymbol{t}$$

MC samples

$$F(\boldsymbol{t}) = A(t_n, t_1) \prod_{k=1}^{n-1} B(t_k, t_{k+1})$$

Data

$$A(t, t') = \langle \psi(t) | O | \psi(t') \rangle$$

$$B(t, t') = \langle \psi(t) | \psi(t') \rangle$$

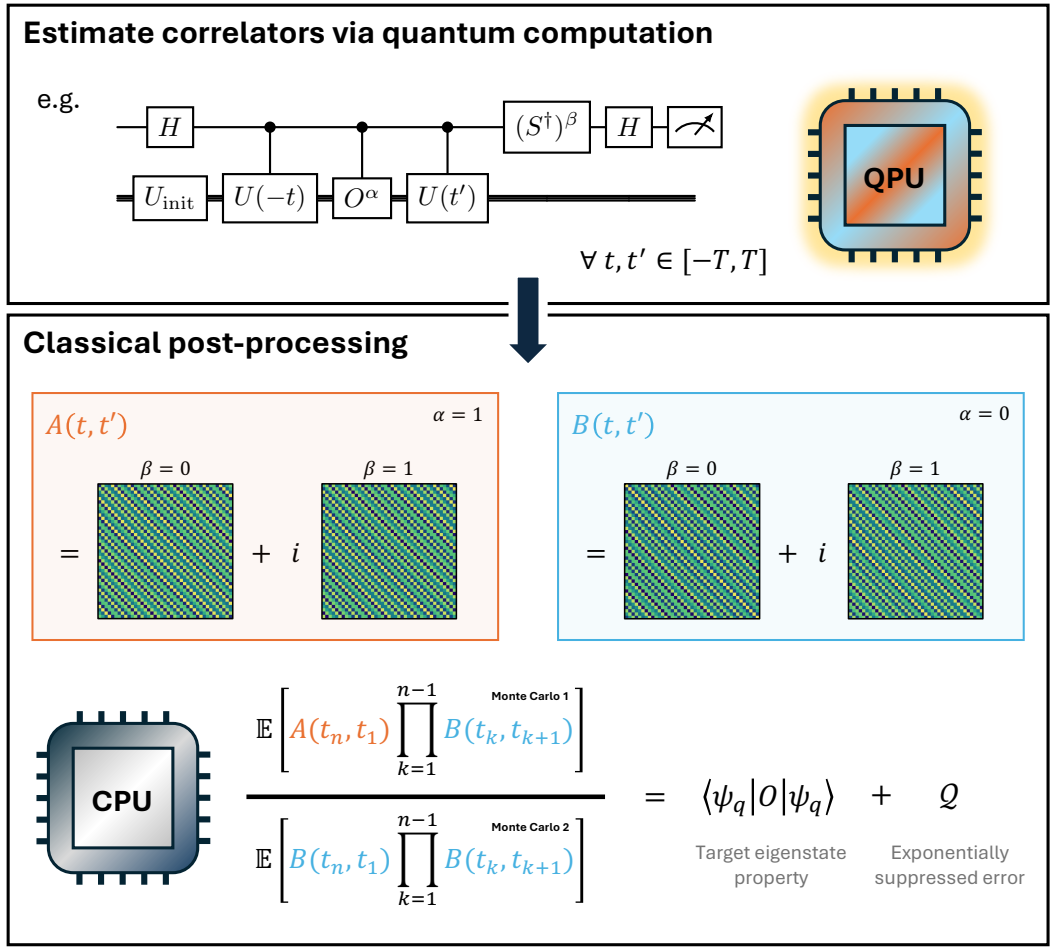
$$\mathrm{Tr}[\bar{\rho}^n] = \int G(\boldsymbol{t}) J(\boldsymbol{t}) \mathrm{d}\boldsymbol{t}$$

MC 2

$$J(\boldsymbol{t}) = B(t_n, t_1) \prod_{k=1}^{n-1} B(t_k, t_{k+1})$$

MC samples

# DDE algorithm workflow




**Steps:**

1. **Quantum computation**:
   a. Choose **temporal grid** cutoff *T* and timestep *dt*.
   b. Estimate **A and B objects** on the 2D timegrid using a quantum device.
2. **Generate MC samples**:
   a. Discretize Gaussian **PDF for the gridpoints**.
   b. Sample *2n* **timepoints** from the discretized PDF for each MC sample.
   c. Calculate the corresponding ***F* and *J* objects**.
3. **Estimate expectation value**:
   a. Using the MC samples estimate the **numerator** and **denominator**.
   b. Take the **ratio** of the estimates.

# Exact simulation:

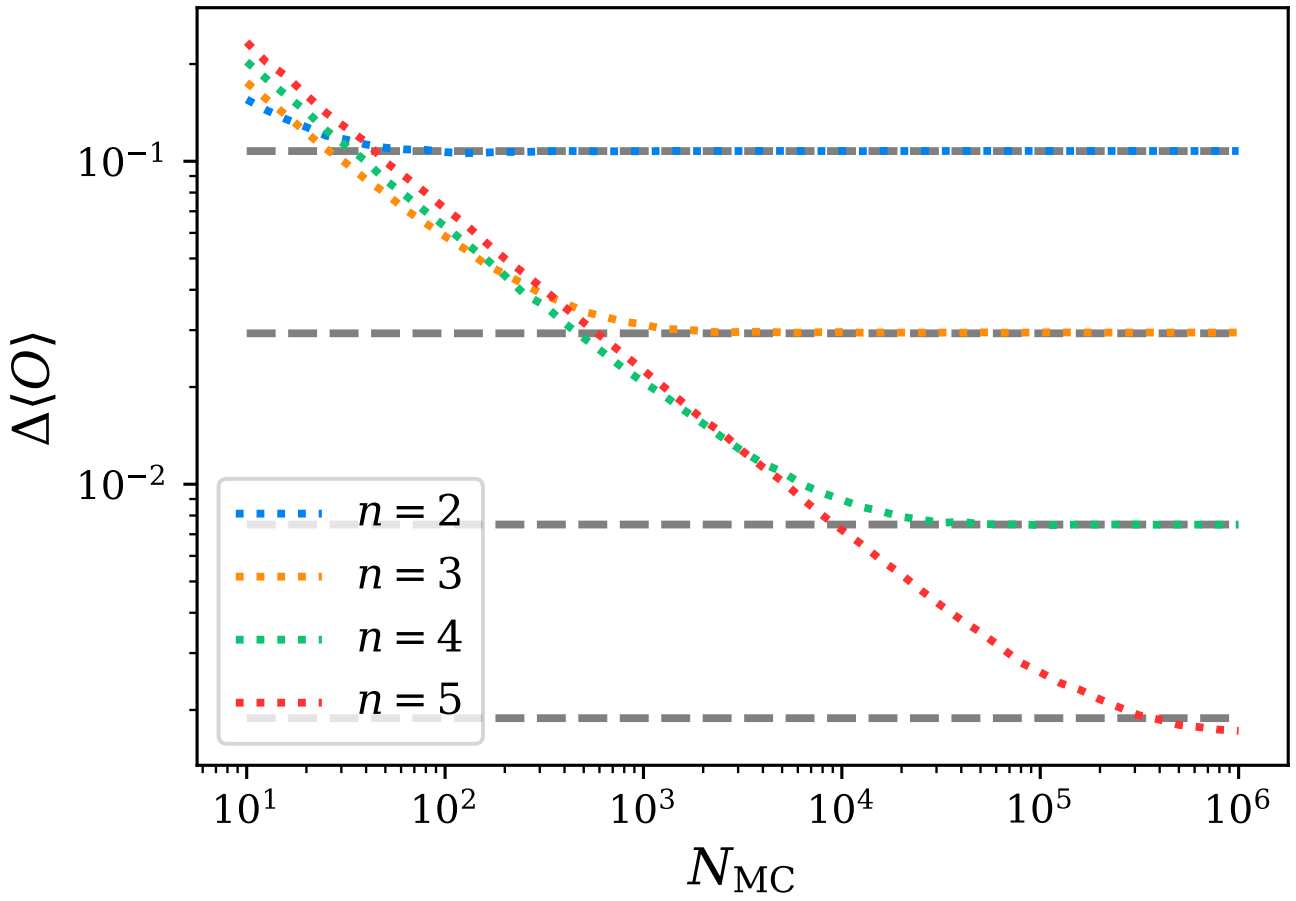
## Random-field Heisenberg model

- Hamiltonian (10 qubits):

$$\mathcal{H} = J \sum_{j=1}^{N} \vec{S}_j \cdot \vec{S}_{j+1} \sum_{j=1}^{N} h_j Z_j$$

  with periodic boundary condition
- Input state:
  - $p_1 = 0.66$
  - $p_k = p_l = 0.17$
- Observable: $O = Z_1$
  - Goal: estimate $\langle \psi_1 | Z_1 | \psi_1 \rangle$

- $T = 200$
- $\sigma = 50$
- $\mathrm{dt} = 0.5$



# Early fault-tolerance:
## Fermi-Hubbard model

**Motivation**: It is expected that early fault-tolerant machines will enable simple Hamiltonian simulation algorithms such as **Trotterization**.

- Hamiltonian:

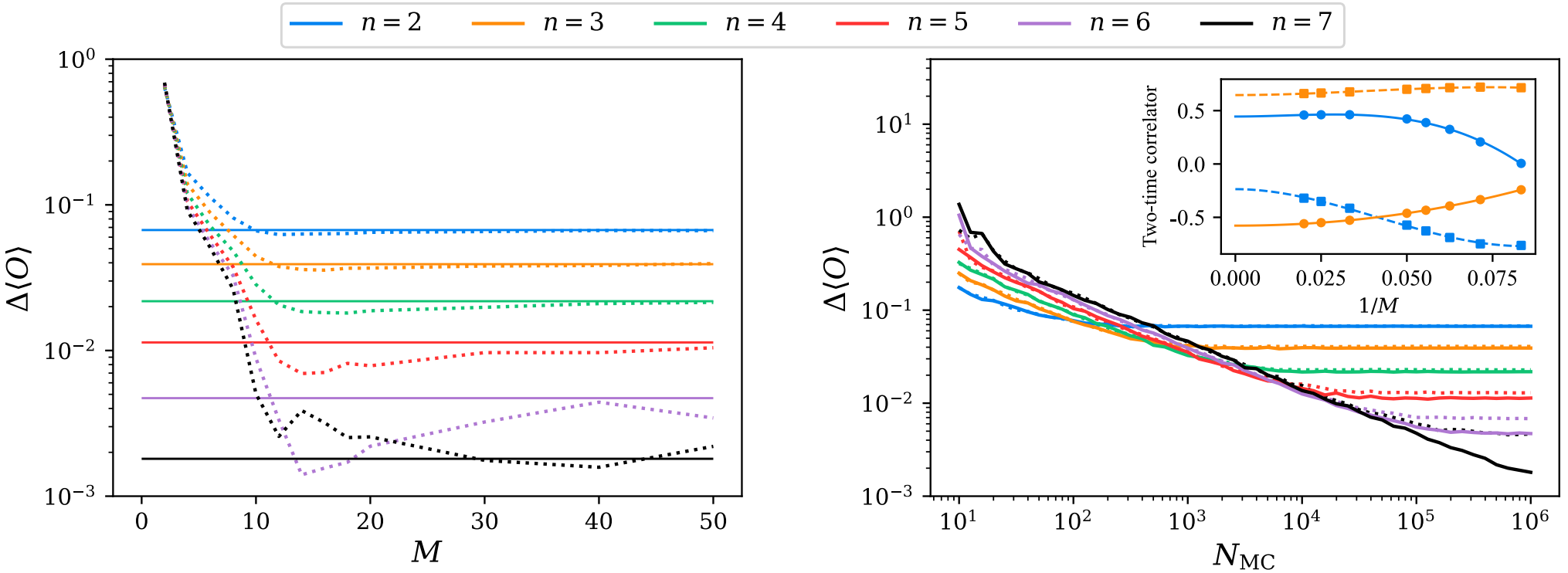
$$\mathcal{H} = -t \sum_{\langle i,j \rangle, s} \left( c_{i,s}^{\dagger} c_{j,s} + c_{j,s}^{\dagger} c_{i,s} \right) + U \sum_{i} n_{i\uparrow} \, n_{i\downarrow}$$

  Interacting fermions on a 2x2 lattice with PBC
  4-site system mapped to **8 qubits** with Jordan-Wigner
- Input state: lowest energy state in the 4 spin subspace
  - $p_1 = 0.62$
- Observable: $O = Z_1 Z_2$
  - Goal: estimate $\langle \psi_1 | Z_1 Z_2 | \psi_1 \rangle$

- $T = 200$
- $\sigma = 50$
- $\mathrm{dt} = 0.5$

# **Early fault-tolerance:**
## Fermi-Hubbard model

**Robustness to Trotter error**

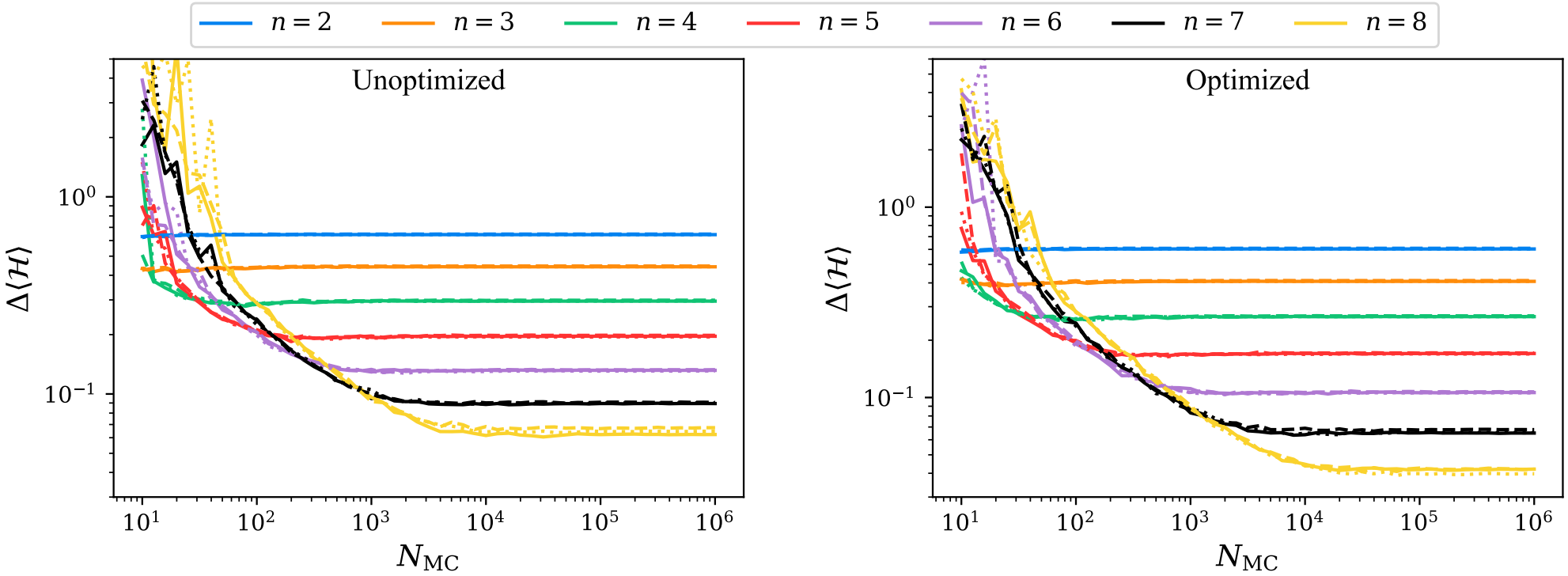


# Early fault-tolerance:
## Fermi-Hubbard model

- Observable: $O = \mathcal{H}$

**Robustness to gate noise**

(noisy rotation gates due to Clifford+T synthesis)




Optimized construction exploits that $O$ commutes with the Hamiltonian.

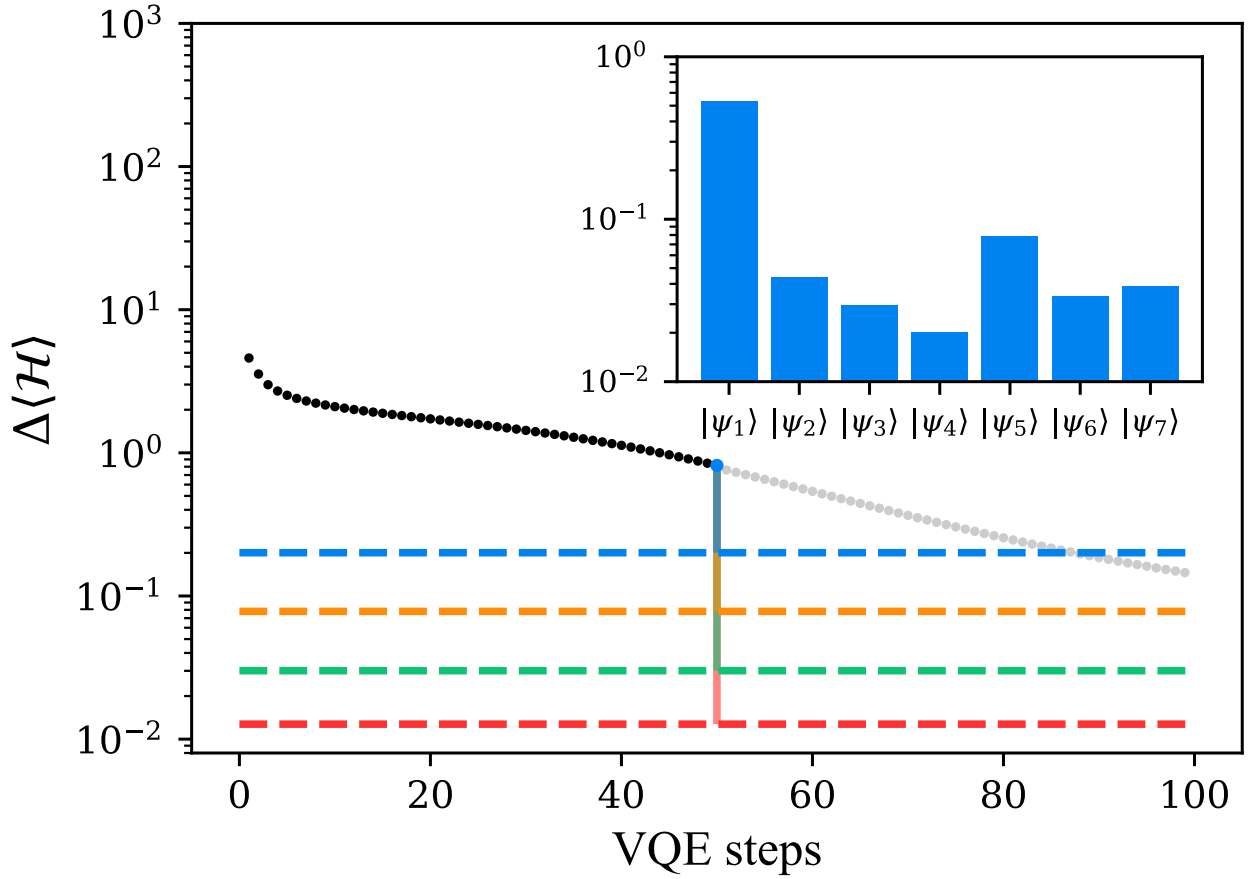
Average number of errors in time evolution: 0, 0.1, 0.01

# Near-term simulation:
## Lattice Schwinger model

**Variational real time evolution**

- Hamiltonian (6 qubits): toy model from high energy physics
  $\mathcal{H} = \mathcal{H}_{ZZ} + \mathcal{H}_{\pm} + \mathcal{H}_{Z}$
- Input state: from VQE
  - $p_1 = 0.53$
- Observable: $O = \mathcal{H}$
  - Goal: estimate $\langle\psi_1|\mathcal{H}|\psi_1\rangle$ (ground state energy)

- $T = 50$
- $\sigma = 12.5$
- $\mathrm{dt} = 0.2$

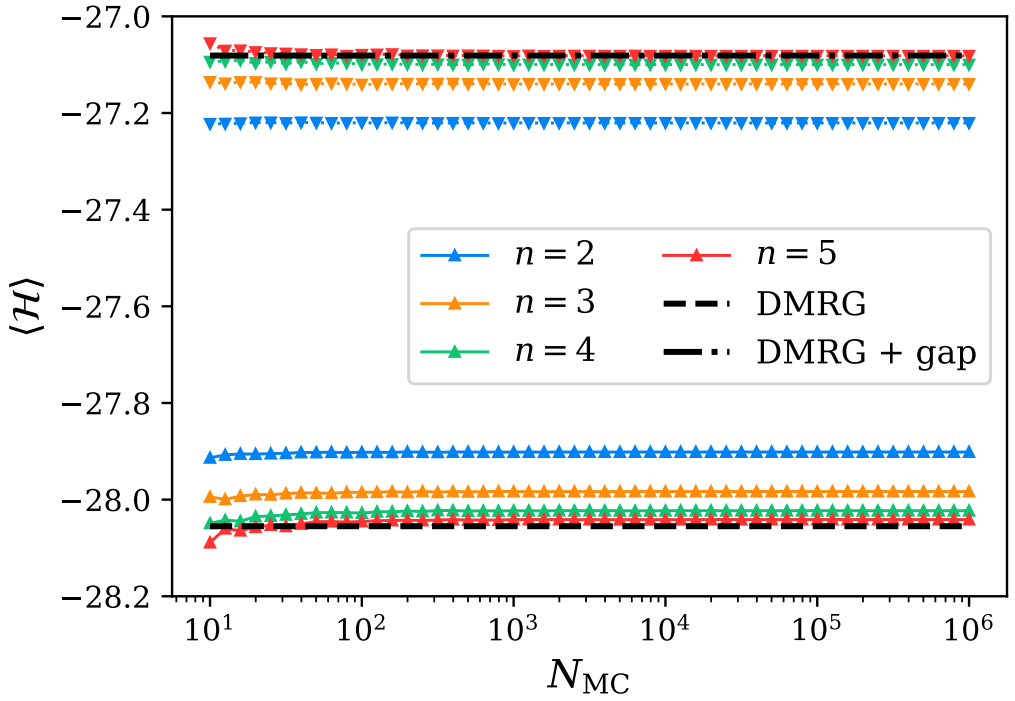


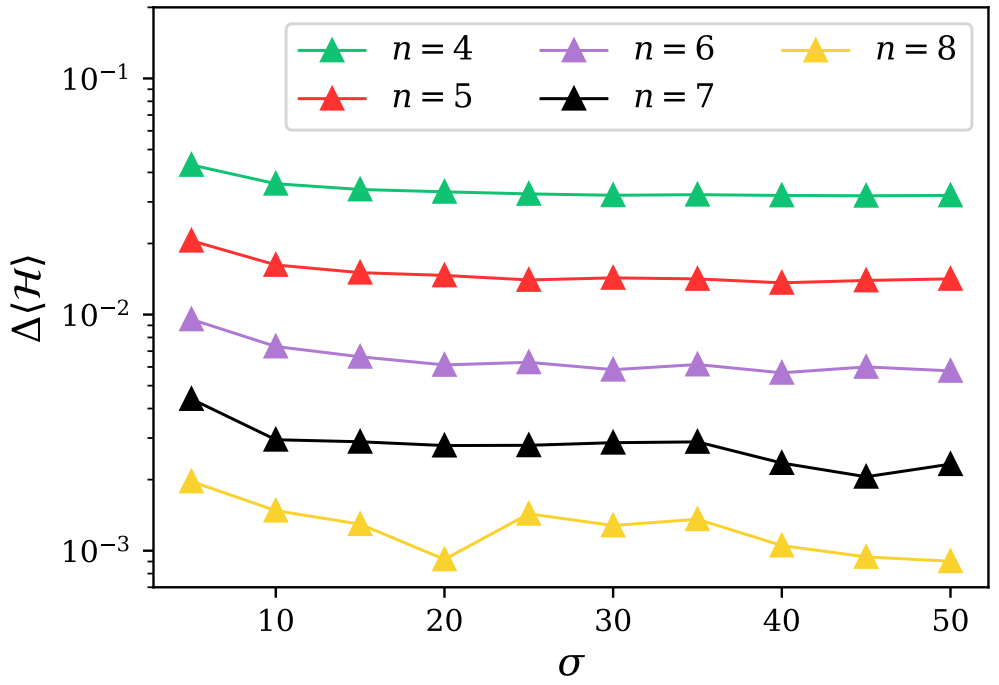
# **Quantum-inspired implementation**: Random-field Heisenberg model

- **Motivation**: Our algorithm is compatible with **quantum-inspired** approaches as well, such as **tensor network** methods.

- In our implementation:
  - **Initial state**: matrix product state (**MPS**).
  - **Time evolution**: **TEBD** algorithm.
  - **Obtaining A and B correlators**: tensor contractions.
  - **Goal**: ground state and excited state energy.
  - Similar hyperparameters as before.

# 100-qubit MPS simulation:
## Random-field Heisenberg model



HUN REN | Wigner

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# Thank you!

Soon on arXiv!

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