

// YQIS – Paris INRIA

Early Fault-Tolerant Quantum Algorithms in Practice

Oriel Kiss,
November 6th, 2024

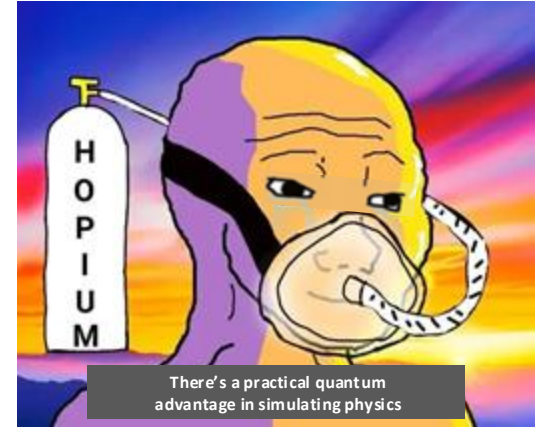
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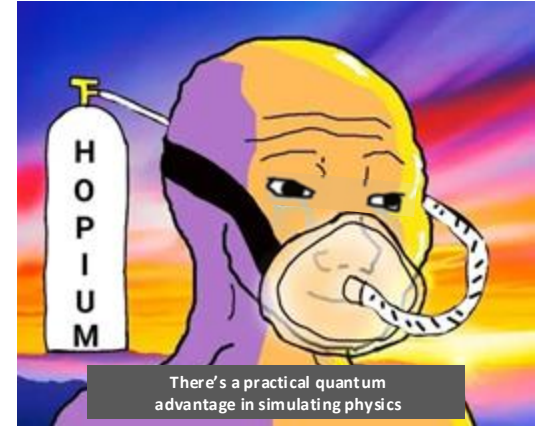
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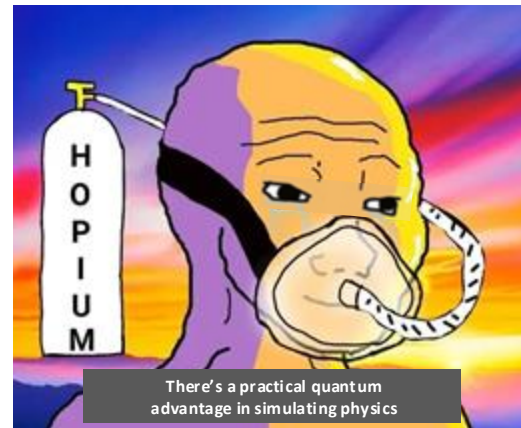
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NISQ

Variational Algorithms
(VQE, QAOA)

No theoretical arguments
for quantum advantage

Scaling - ϵ^{-2}



There's a practical quantum advantage in simulating physics

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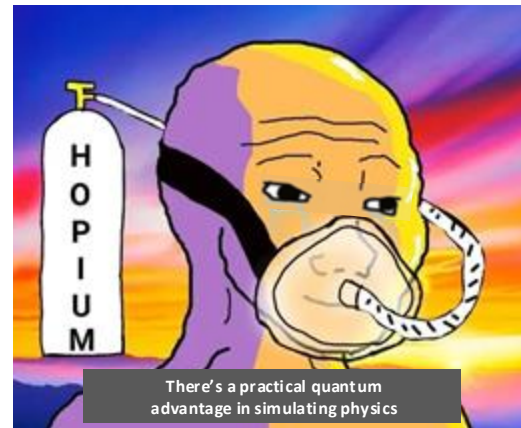
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Fully-FTQC

Phase Estimation
(QPE, QETU, filters, ...)

T-gate counts,
High-depth
Coherent computation

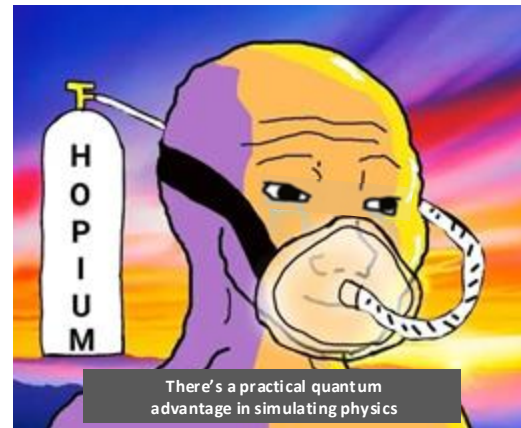
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Prefactor matters!

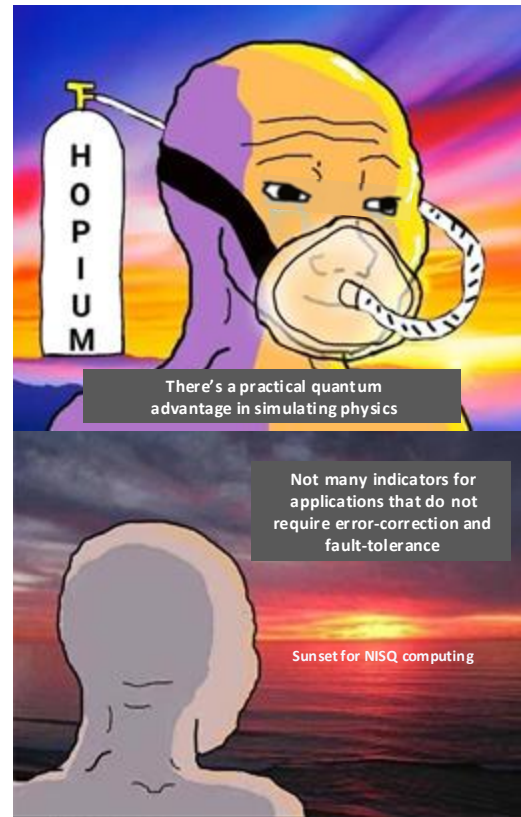
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// Overview

1. Early fault-tolerant algorithms for GSEE: review of the Lin&Tong algorithm.
2. Applying the Lin&Tong algorithm in practice.
3. Numerical simulations.
4. Bonus: application on NISQ devices.

// Early-FTQC Algorithms for GSEE

Find the lowest eigenvalue of a **Hamiltonian H** describing a system with some error ϵ ,

$$\tau H = \sum_k \tau_k |E_k\rangle\langle E_k| \text{ with } \|\tau H\| < \pi/2$$

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2. The circuit depth is short, ideally $O(\epsilon^{-1})$ (Heisenberg scaling).
3. Some degree of robustness against algorithmic errors.

// The Lin-Tong Algorithm

Problem 1. *Given a precision $\delta > 0$ and lower bound on the overlap parameter $\eta > 0$, we seek to decide if*

$$\text{Tr}[\rho\Pi_{\leq x-\delta}] < \eta \quad \text{or} \quad \text{Tr}[\rho\Pi_{\leq x+\delta}] > 0. \quad (3)$$

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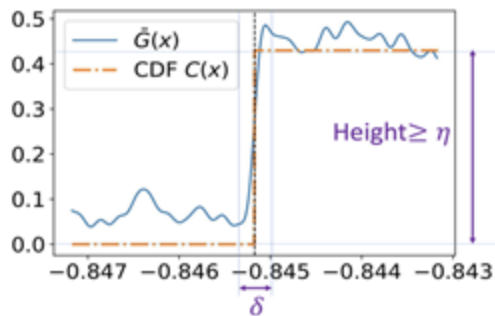
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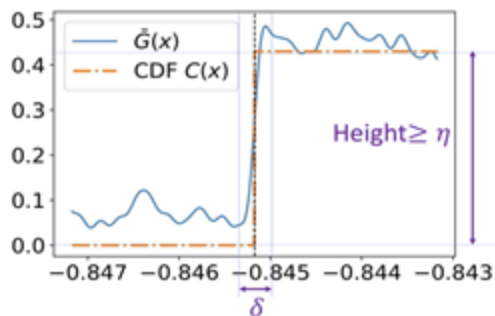
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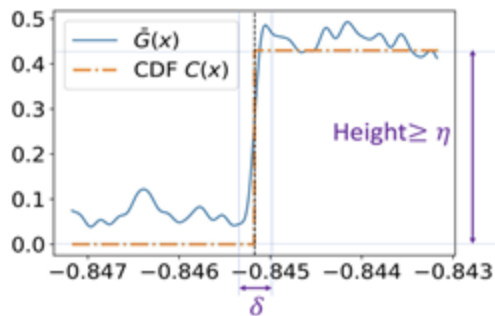
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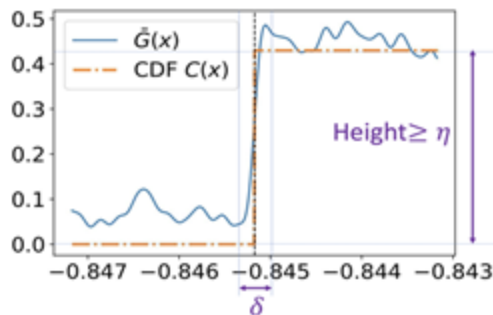
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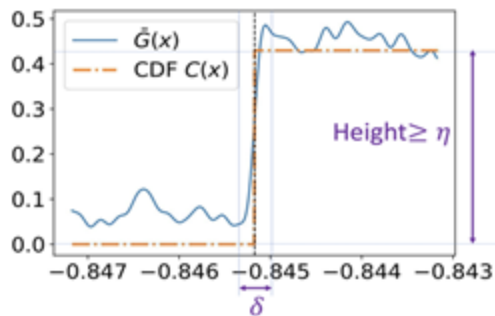
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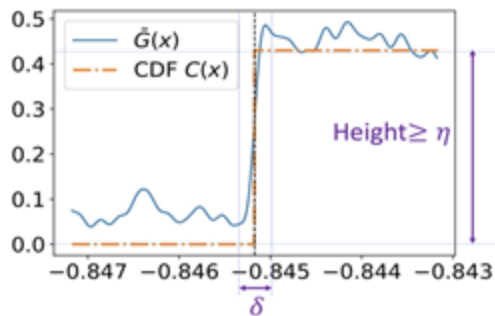
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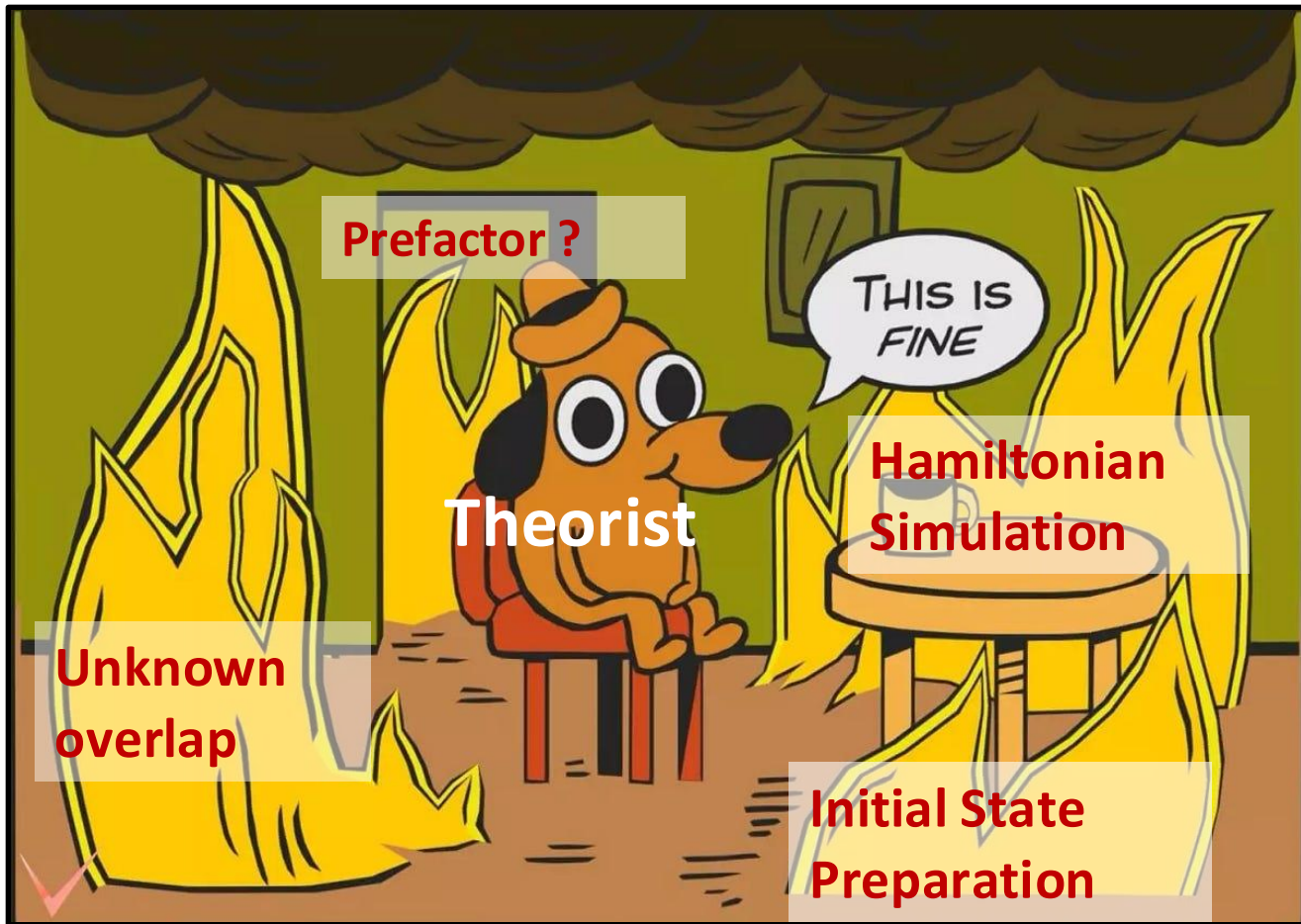
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$$G(x) = \frac{1}{2} + \frac{2\mathcal{F}}{M} \sum_{i=1}^M \left[\text{Re}[g_{k_i}(\tau)] \sin(k_i x) + \text{Im}[g_{k_i}(\tau)] \cos(k_i x) \right].$$



Prefactor ?

THIS IS
FINE

Theorist

Hamiltonian
Simulation

Unknown
overlap

Initial State
Preparation

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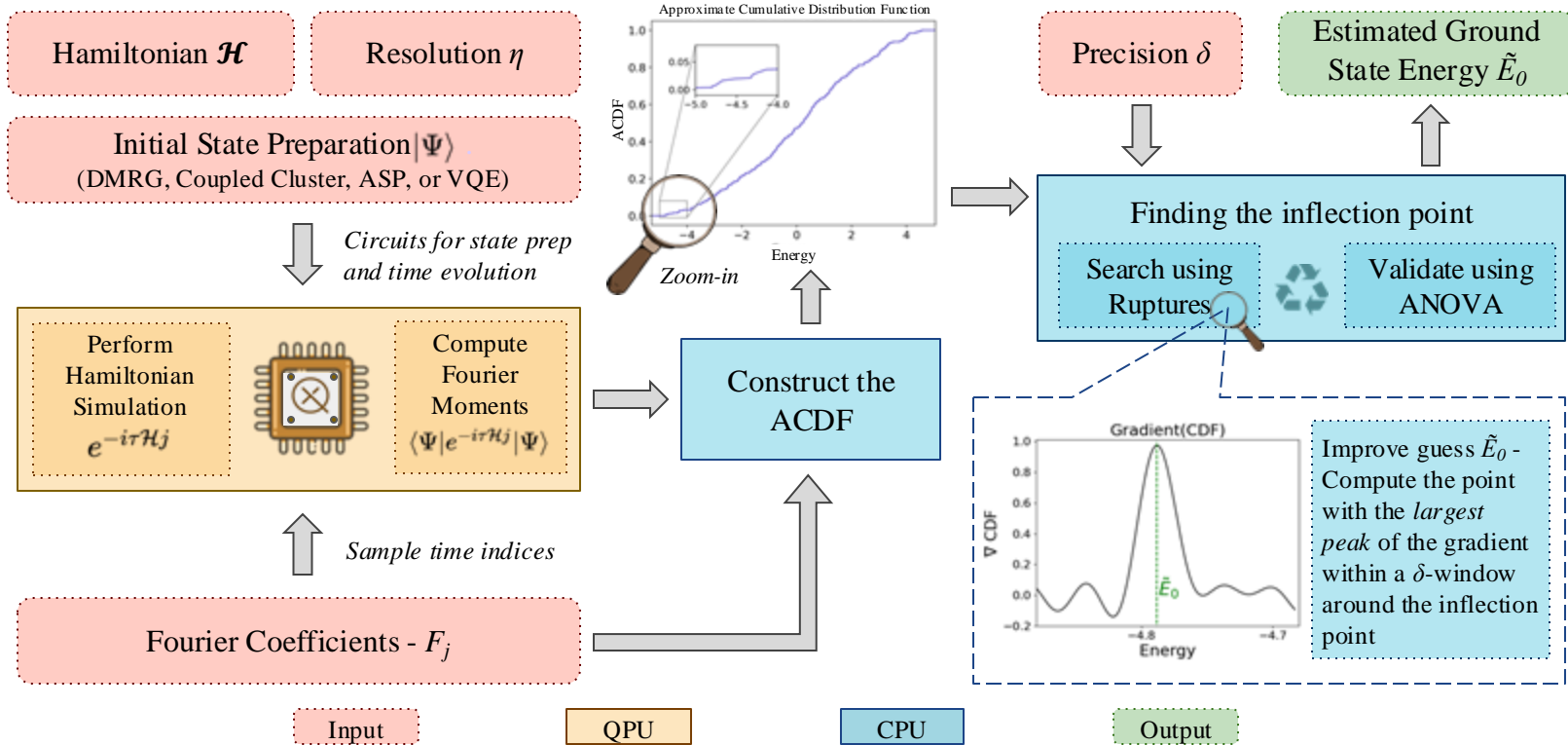
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- 🔧 **Hamiltonian Simulation:** **system-specific**; we use (asymptotical sub-optimal) product formula because:

1. no ancilla overhead
2. take advantage of locality
3. often much better than what is guaranteed
4. can scale better than qubitization in some regime



// Our Workflow

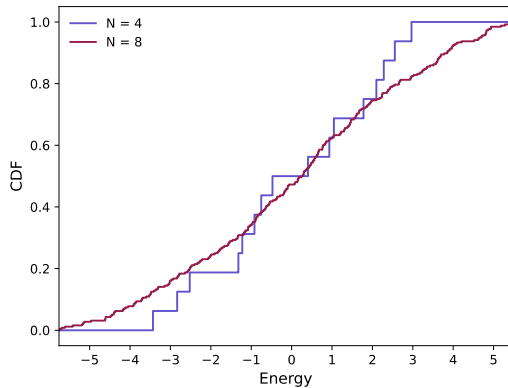


// Key Insights I: Find Inflection

CDF smoothes out with the system size (random initial state)

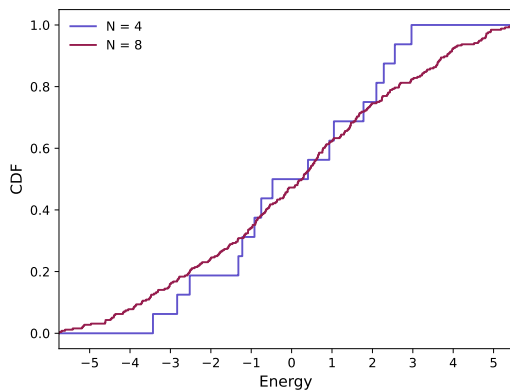
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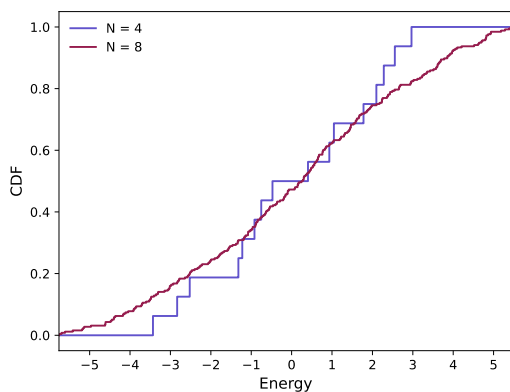
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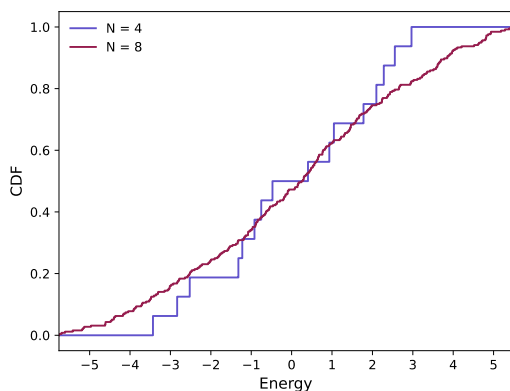
XXZ model

Search a
breakpoint

$$\min_{b \in \{1, \dots, n\}} \sum_{t=1}^b \|\phi(y_t) - \bar{y}_{1:b}\| + \sum_{t=b+1}^n \|\phi(y_t) - \bar{y}_{b+1:n}\|,$$

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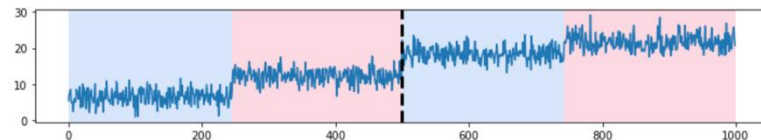
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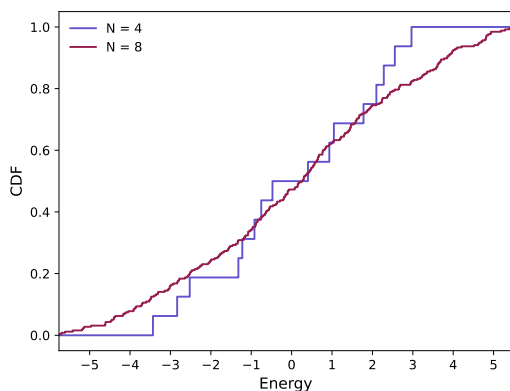
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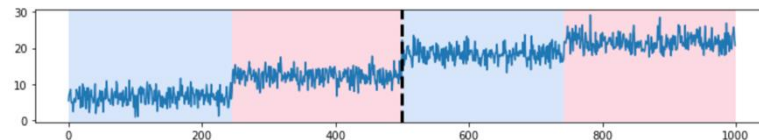
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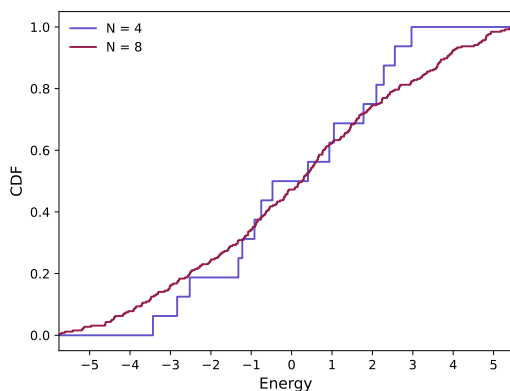
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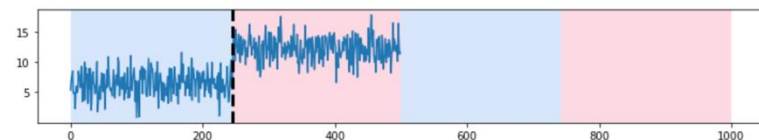
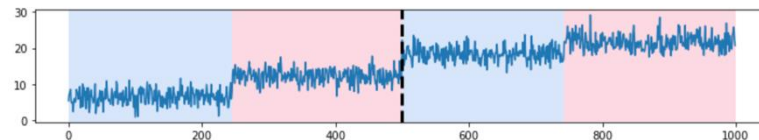
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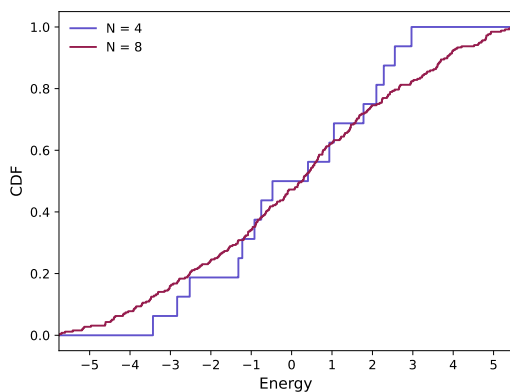
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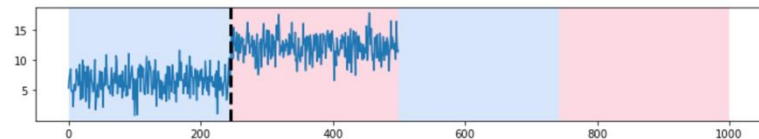
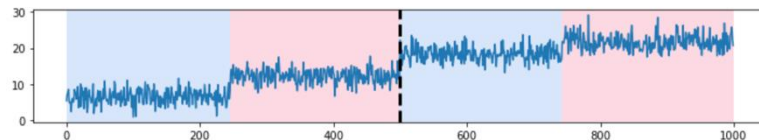
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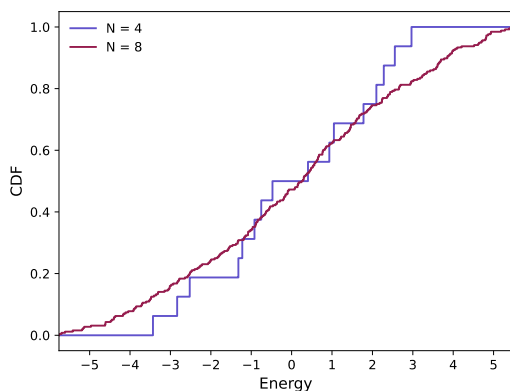
Validate the
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Use ANOVA to test the statistical significance using F-test



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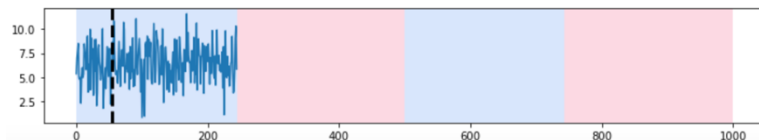
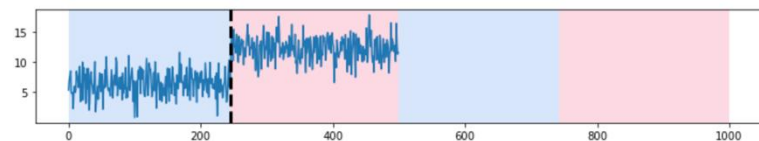
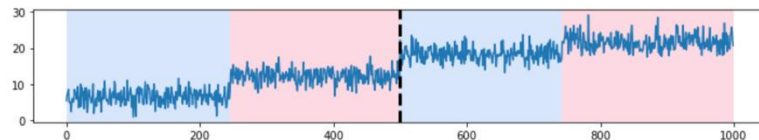
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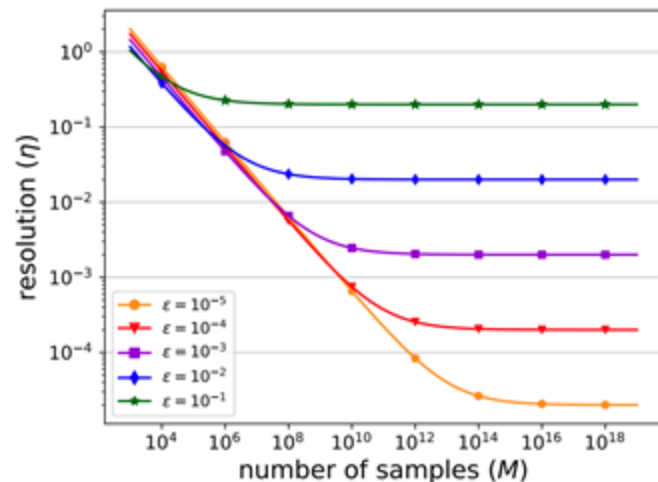
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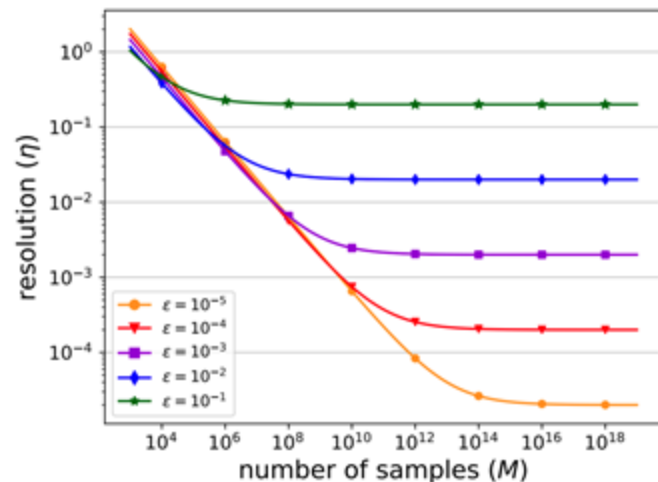
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To resolve bad initial states, we require more depth (and not only samples).

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// Numerical Simulations

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$$\mathcal{H} = \frac{1}{N} \sum_{i < j} \sum_{a \in \{x, y, z\}} J_a^{ij} \cdot \sigma_a^i \sigma_a^j, \text{ where } J_a^{ij} \sim \mathcal{N}(0, 1).$$

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$$\mathcal{H} = \frac{1}{N} \sum_{i < j} \sum_{a \in \{x, y, z\}} J_a^{ij} \cdot \sigma_a^i \sigma_a^j, \text{ where } J_a^{ij} \sim \mathcal{N}(0, 1).$$

Why? : universal, long-range, challenging for DMRG.

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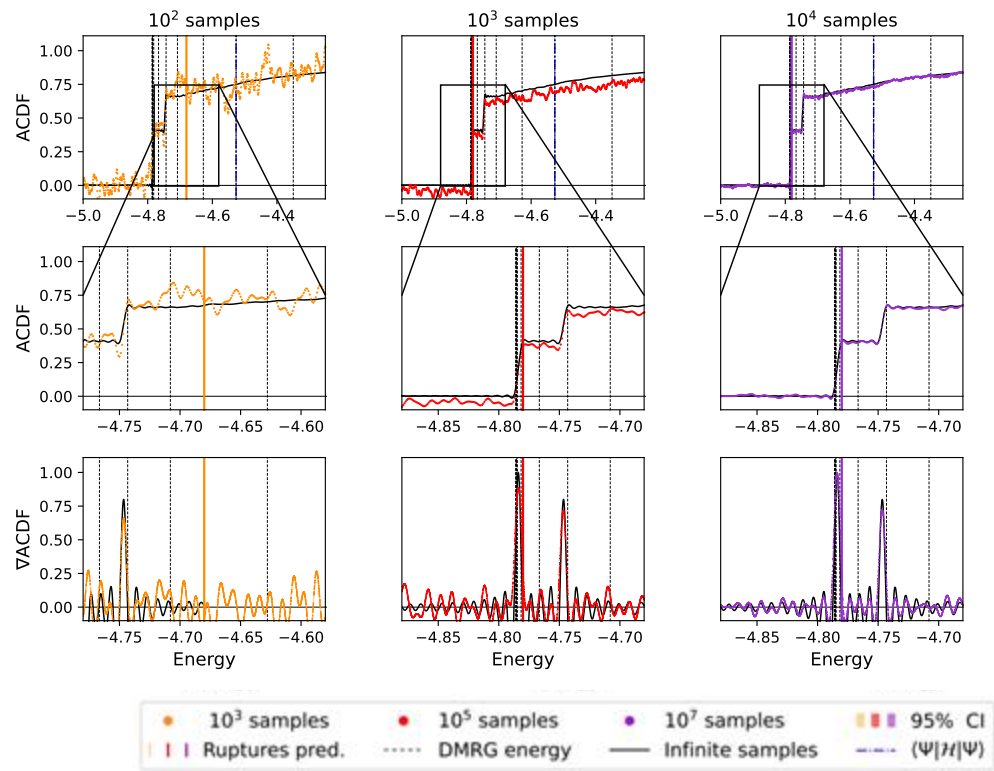
For dynamics, we use a **second-order Trotter-Suzuki** with time step $\Delta t = \tau/8$.

The circuit construction is based on SWAP networks.

We look at **$N=26$** spins,

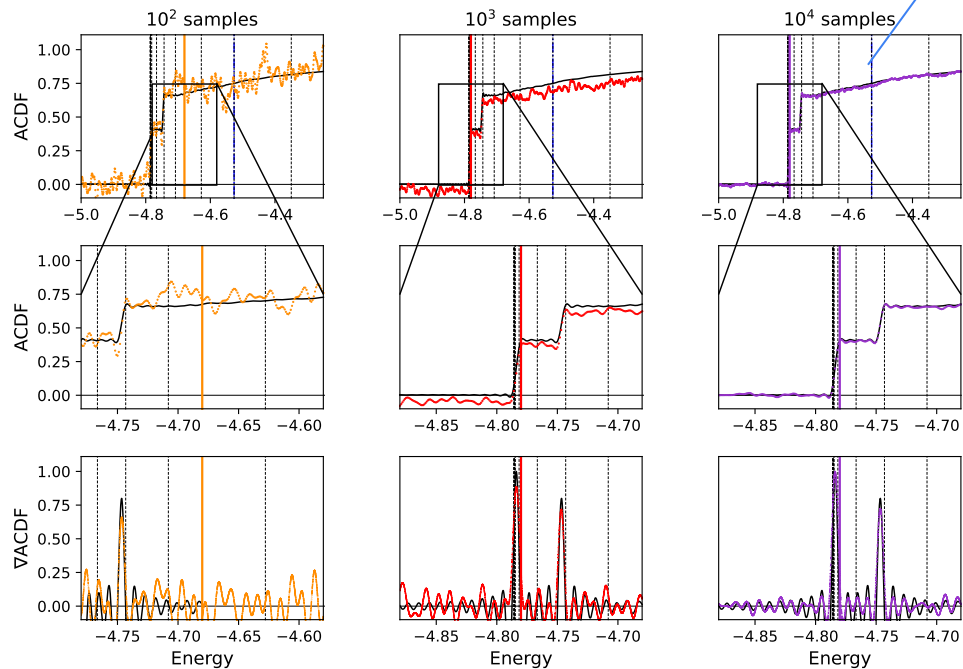
and use initial states prepared via DMRG (with low bond dimension).

// Key Insights III: DMRG(bd = 10) Initial State



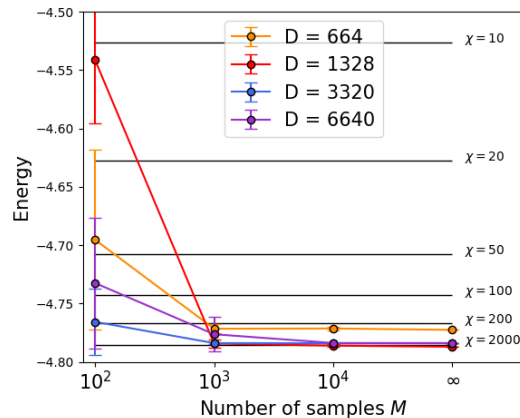
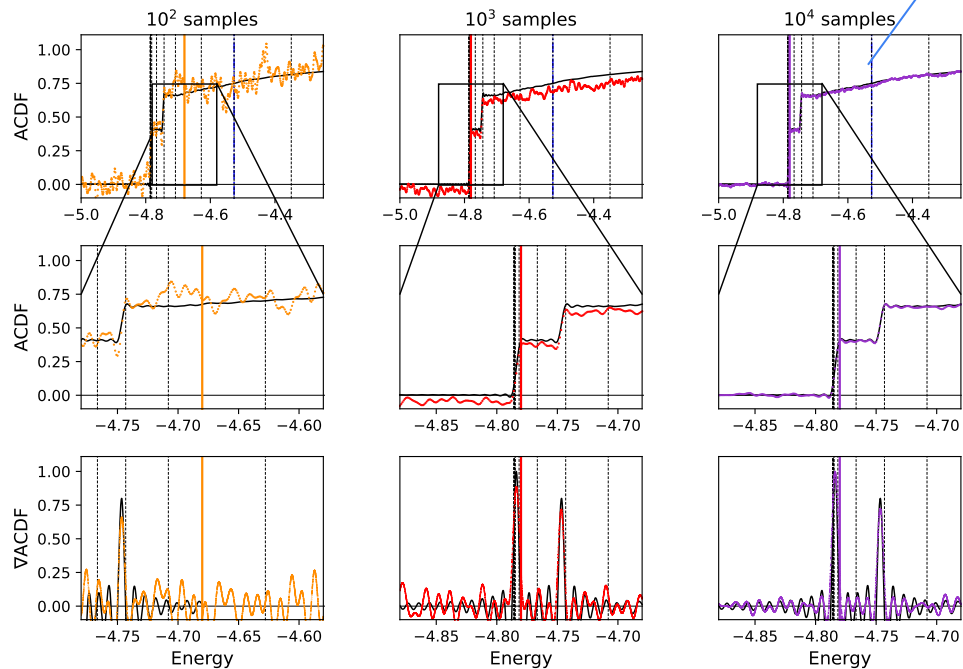
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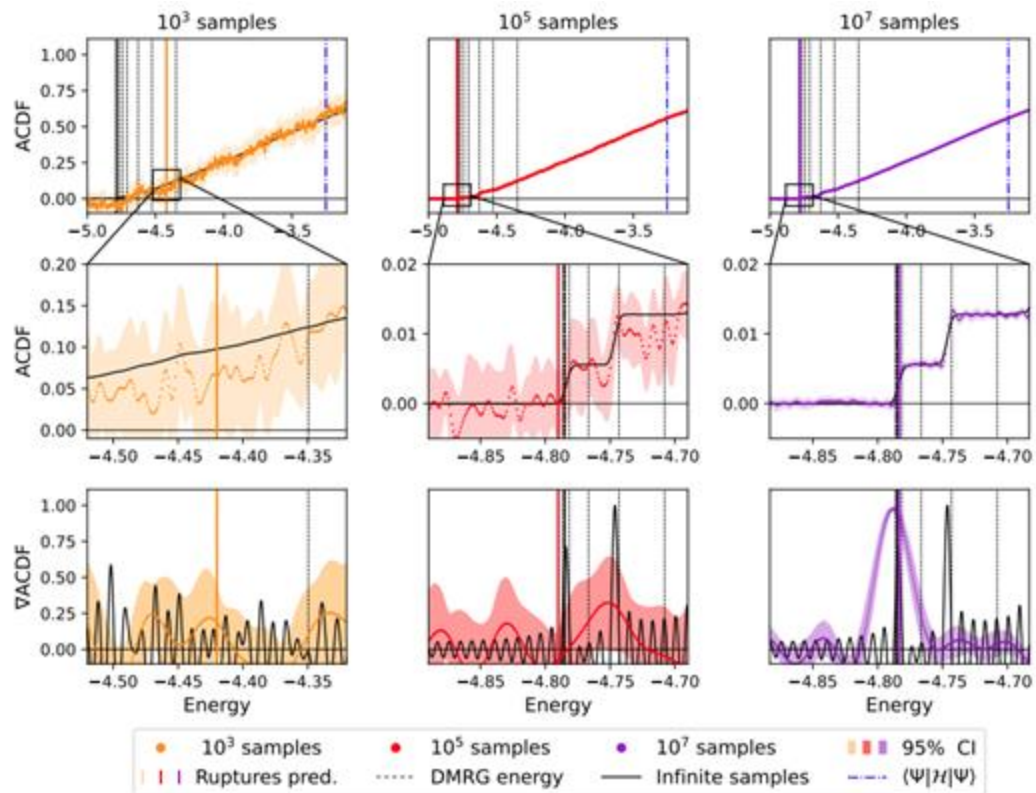


Depth matters most!

$p_0 = 7 \times 10^{-6}$ (overlap)
 $M = 10^{13}$ samples

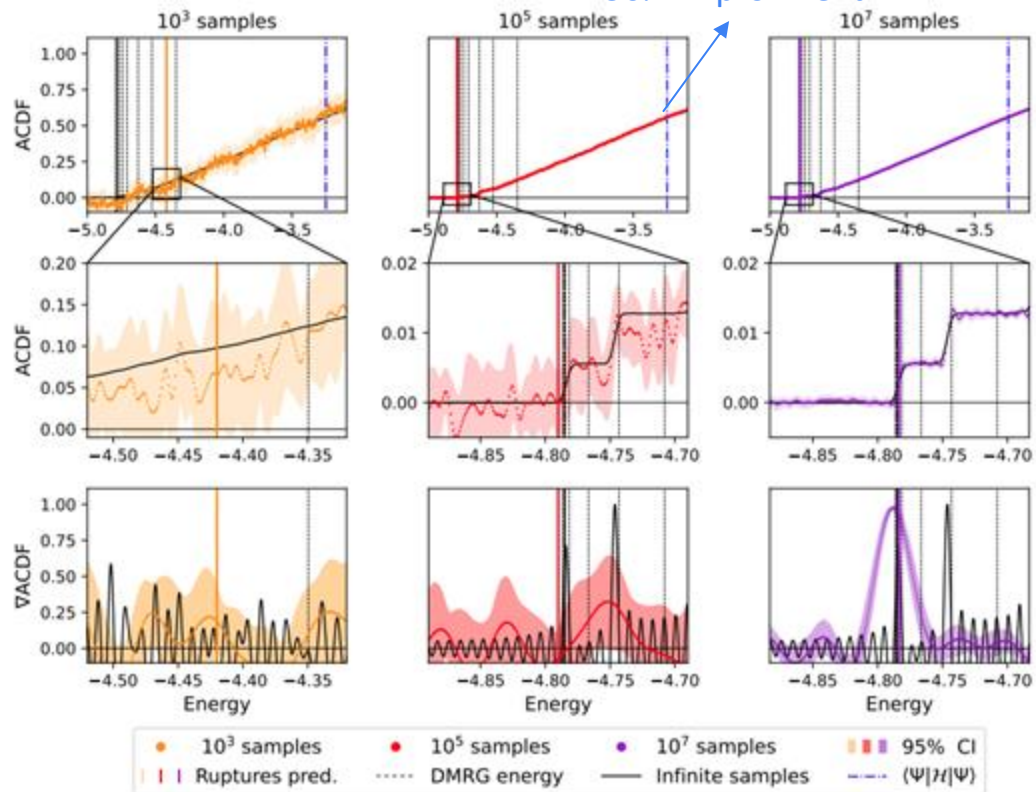


// Key Insights III: Sparsified DMRG



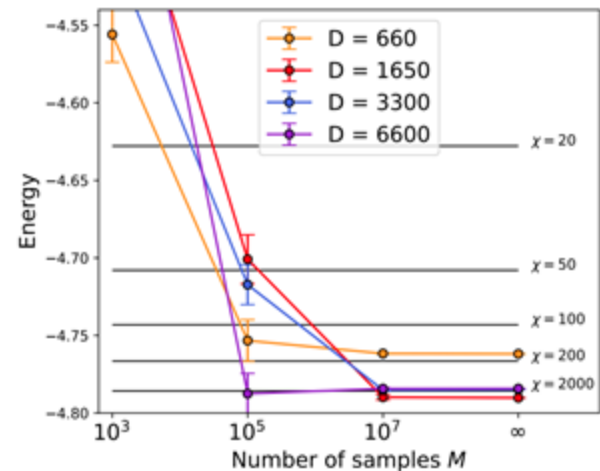
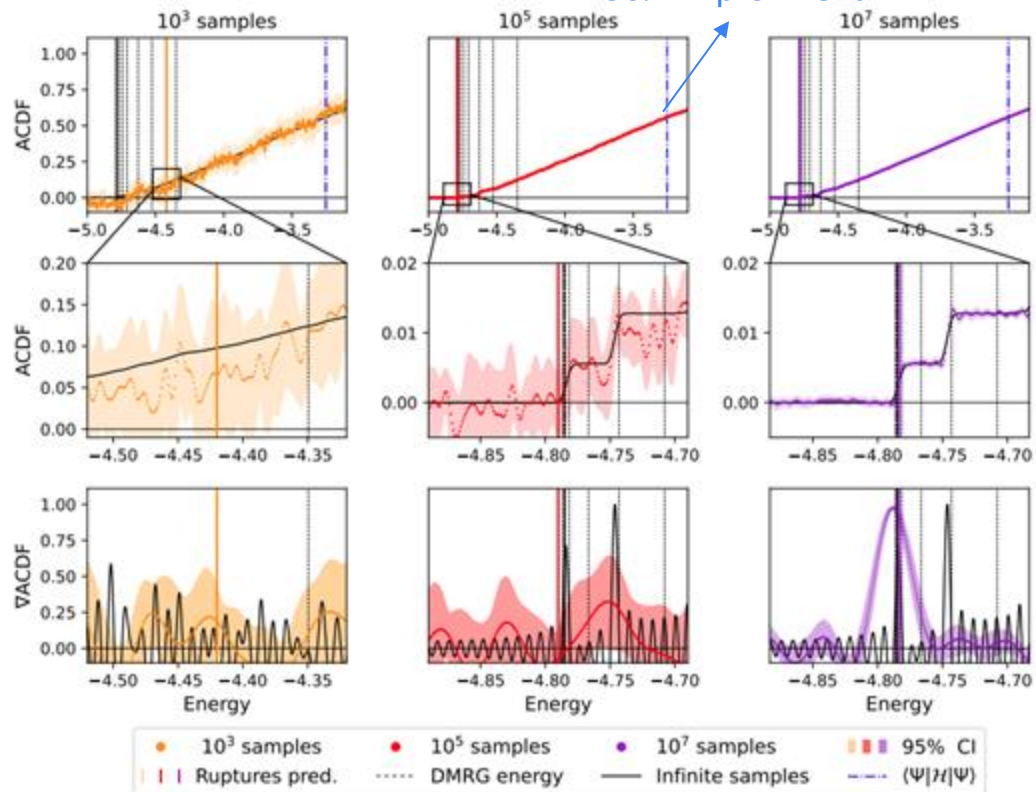
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30% improvement



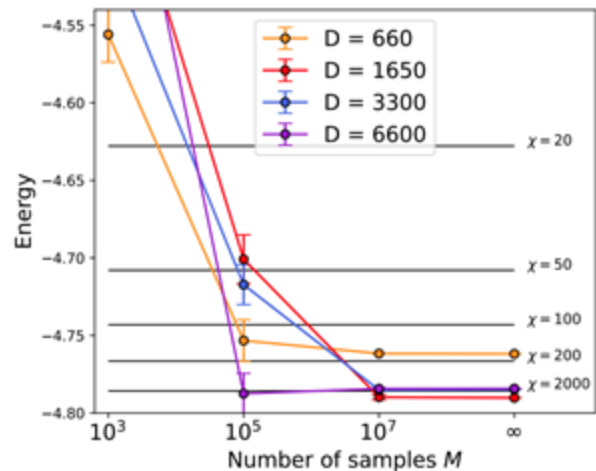
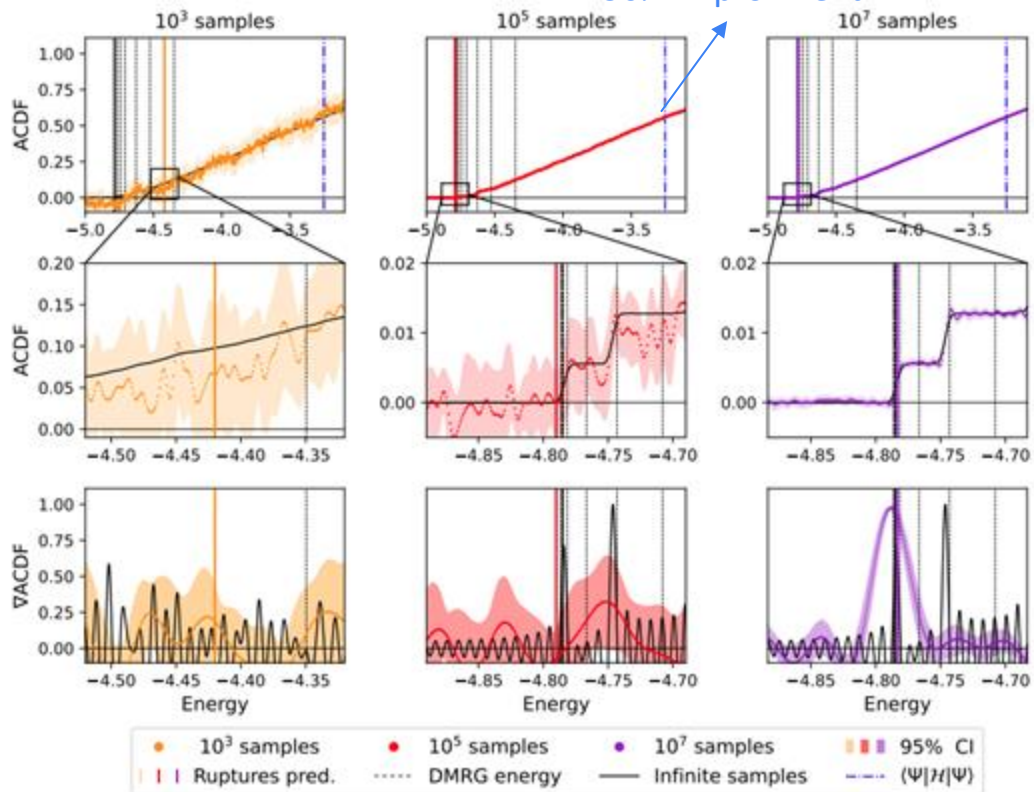
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Fidelity with
initial state
 $p_0 = 2 \times 10^{-5}$

// To Conclude

- .
- .
- .
- .

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// To Conclude

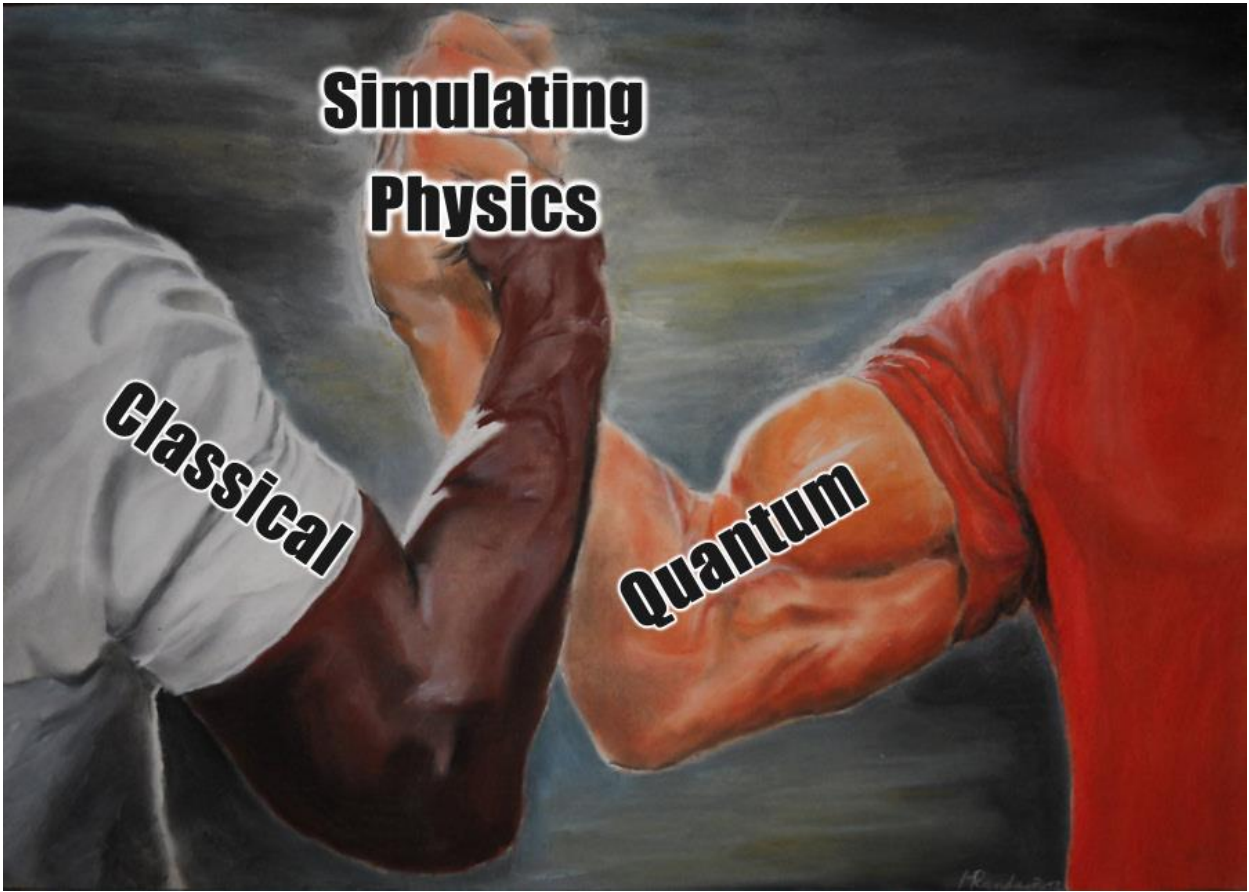
1. LT algorithm (and friends) **bridges** the gap between the NISQ and FTQC eras.
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1. LT algorithm (and friends) **bridges** the gap between the NISQ and FTQC eras.
2. Instead of aiming at the true ground-state energy, one can concentrate on a finding the **inflection point** of the spectral CDF.
3. LT algorithms are able to **improve on classical solutions**, using only limited quantum resources ($\sim 10^5$ samples).
4. If arbitrary precision is required, use quantum phase estimation. However, If a **good approximation is enough**, LT is a robust algorithm, which can be run **in practice**.



// Overview

1. Early fault-tolerant algorithms for GSEE: review of the Lin&Tong algorithm.
2. Applying the Lin&Tong algorithm in practice.
3. Numerical simulations.
4. **Bonus: application on NISQ devices.**

// Bonus: what can we do on NISQ?

- Blunt et al: variational dynamics + ZNE on a H_3 molecule (6 qubits)
- We focus on extracting Fourier moments of a nuclear EFT (4 qubits).

$$\langle \Psi_0 | \hat{O}(\vec{q})^\dagger e^{-iHj\tau} \hat{O}(\vec{q}) | \Psi_0 \rangle$$

- We use **purified echo verification** + various error suppression techniques (twirling, dynamical decoupling, pulse efficient calibration, readout calibration).

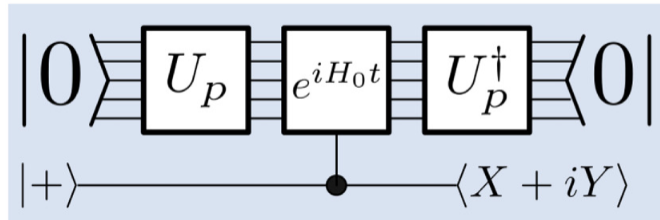


// Purified echo verification

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Verification

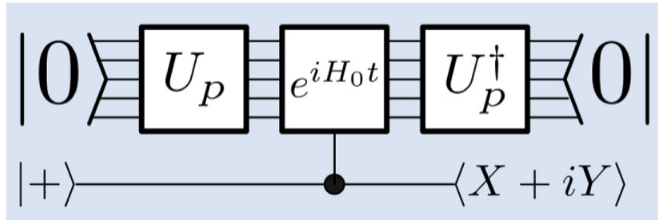
Unprepare the state and verify that it is the zero state



// Purified echo verification

Verification

Unprepare the state and verify that it is the zero state



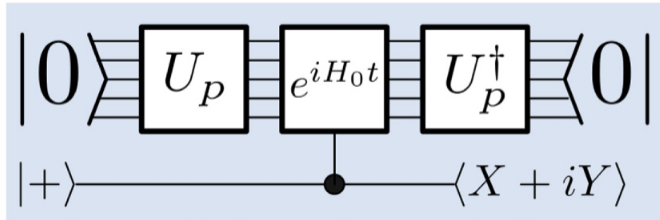
Verification passed \rightarrow state contributes ± 1 to the expectation value.

Otherwise: \rightarrow garbage

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Purification of the ancilla

$$\rho = \lambda |\psi\rangle\langle\psi| + (1 - \lambda) \underbrace{\sum_{k=2}^{2^N} p_k |\psi_k\rangle\langle\psi_k|}_{\text{Noisy components}}.$$

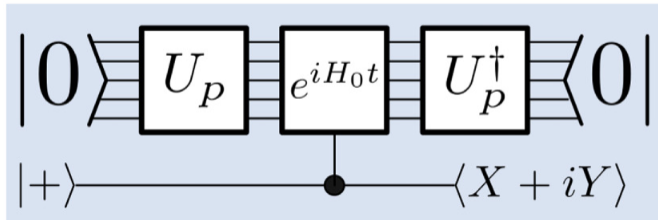
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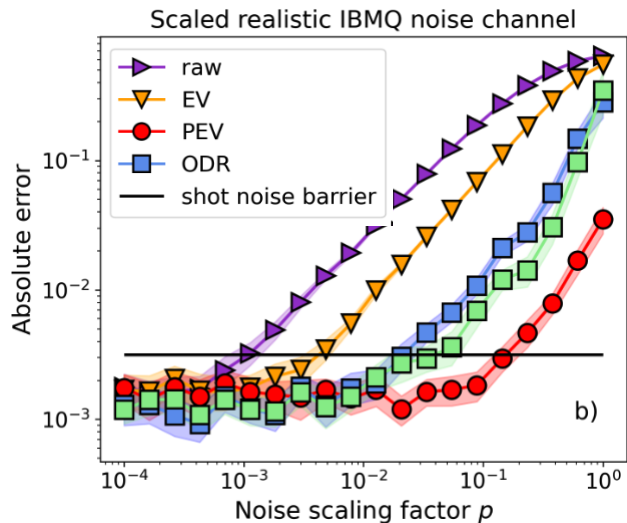
Noisy components

Without noise: the ancilla is pure after post-selection.

With noise: It is not. Extract the closest pure state from measurements.

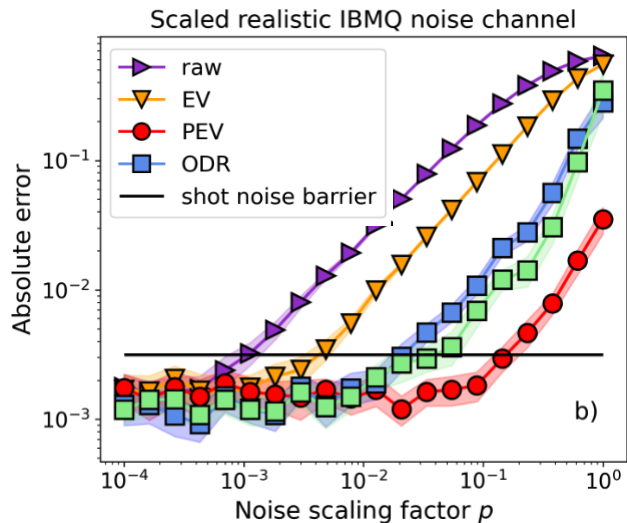
// Results (IBMQ)

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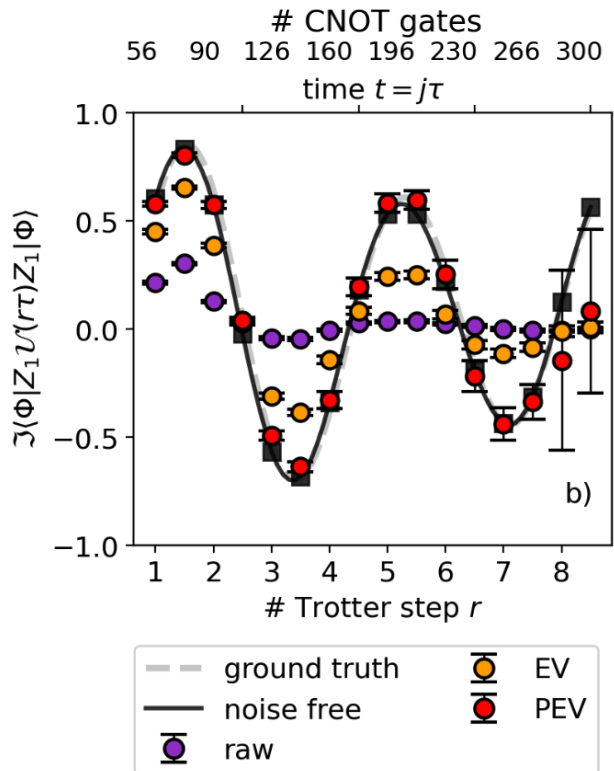


x100 error reduction

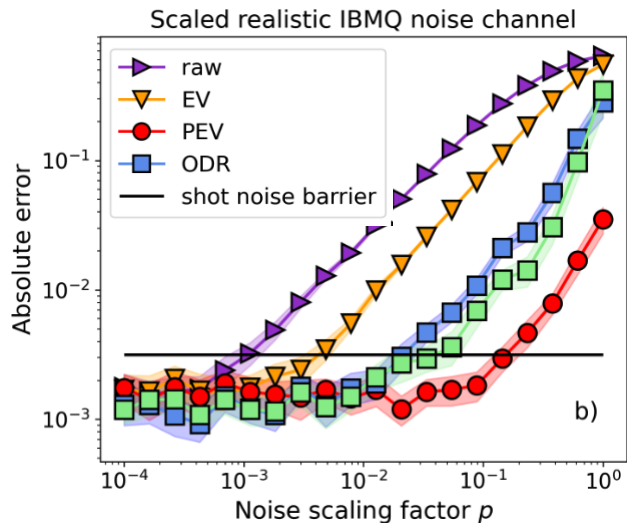
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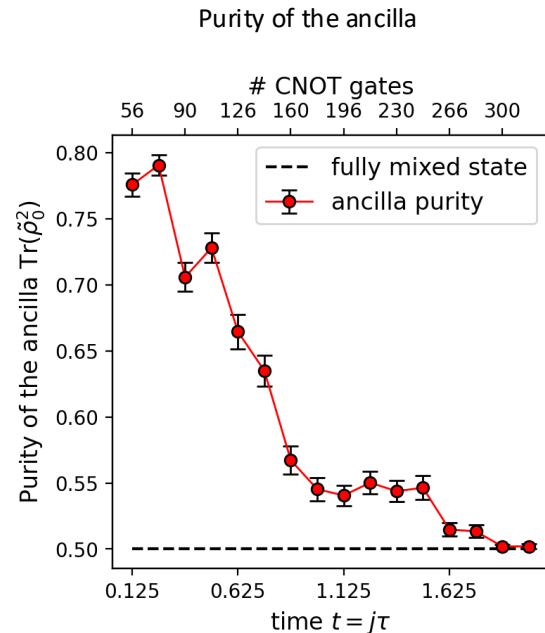
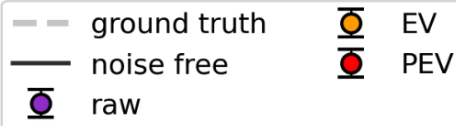
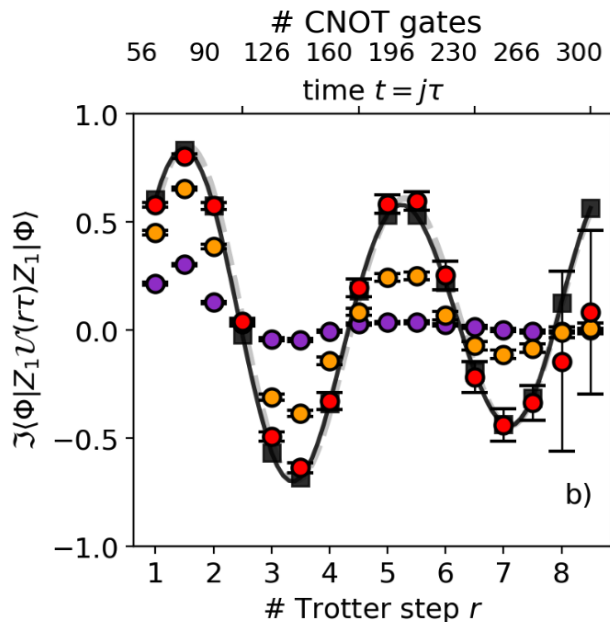
x100 error reduction



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x100 error reduction



We know the breakpoint

Thank You!

// Team



Utkarsh Azad



Borja Requena



David Wakeham



Michele
Grossi



Alessandro
Roggero



Juan Miguel
Arrazola

arXiv:
2405.03754

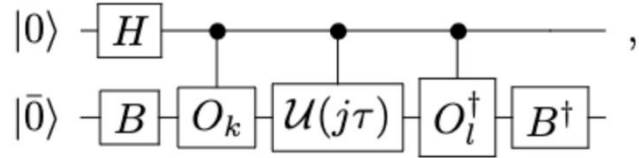


arXiv:
2401.13048



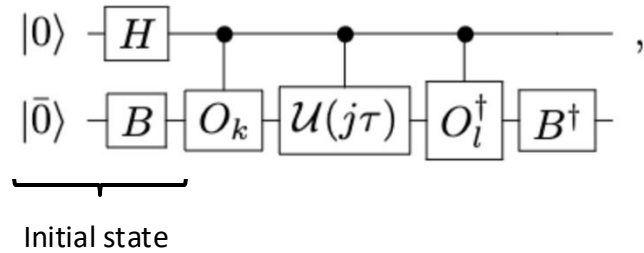
contact: oriel.kiss@cern.ch
twitter: [@oriel_kiss](https://twitter.com/oriel_kiss)

// Purified echo verification (details)



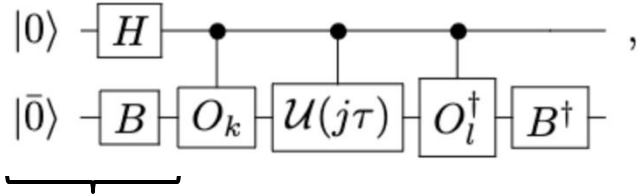
// Purified echo verification (details)

Hadamard test



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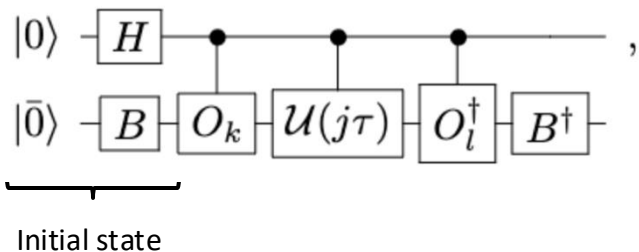
Hadamard test



Initial state

// Purified echo verification (details)

Hadamard test

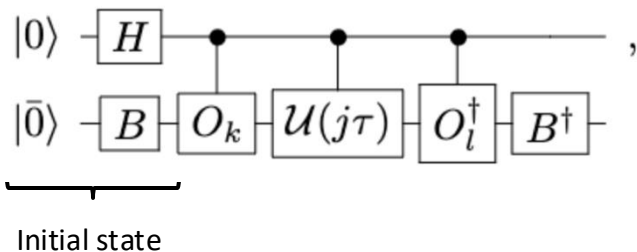


$$|\Phi\rangle = \frac{1}{\sqrt{2}} \left(|\bar{0}\rangle \otimes |0\rangle + B^\dagger O_k^\dagger \mathcal{U}(j\tau) O_l B |\bar{0}\rangle \otimes |1\rangle \right) \\ \equiv \frac{1}{\sqrt{2}} (|\bar{0}\rangle \otimes |0\rangle + |\phi\rangle \otimes |1\rangle),$$

$$|\phi\rangle = \alpha |\bar{0}\rangle + \beta |\bar{0}^\perp\rangle.$$

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Hadamard test



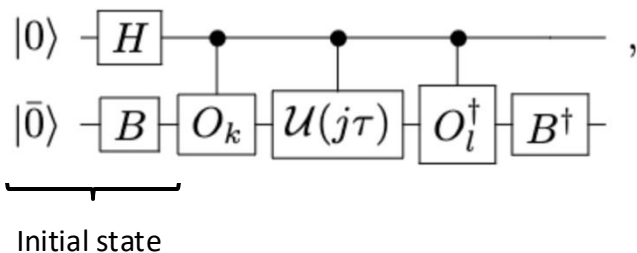
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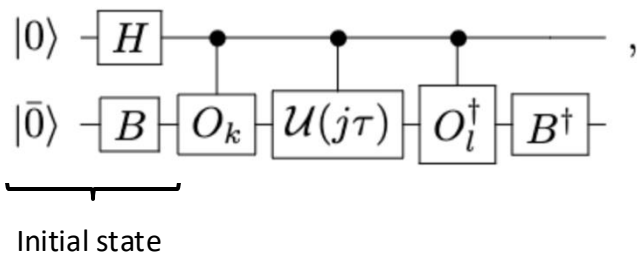
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1. We measure the 3 single-qubit Pauli expectation (X,Y and Z) values of the ancilla.

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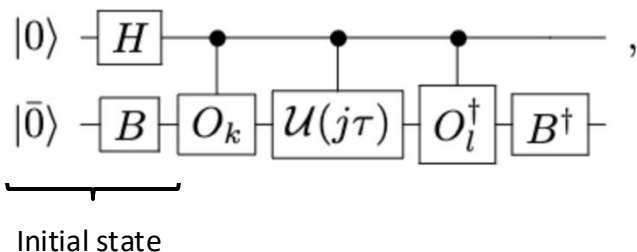
1. We measure the 3 single-qubit Pauli expectation (X,Y and Z) values of the ancilla.

2. Construct the closest compatible pure state (**purification + tomography**).

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$$\text{Re}\{\alpha\} = \frac{\langle X_a \rangle_0}{1 + \langle Z_a \rangle_0}, \quad \text{Im}\{\alpha\} = \frac{\langle Y_a \rangle_0}{1 + \langle Z_a \rangle_0}.$$

// Sparse interpolation via compressive sensing

- Compressive sensing is an optimal technique to recover a signal from few measurements if we know a basis where the signal is sparse.

Theorem 3. Let U be the orthogonal conversion matrix between the measurement basis and the basis where the signal is sparse, with $|U_{k,j}| \leq \mu(U)$. If the number of samples m is chosen such that

$$m \geq C_0 \mu(U)^2 S \log d / \delta \quad (28)$$

$$m \geq C'_0 \log^2 d / \delta, \quad (29)$$

for some constant C_0, C'_0 , then every signal of sparsity S can be recovered with probability $(1 - \delta)$.

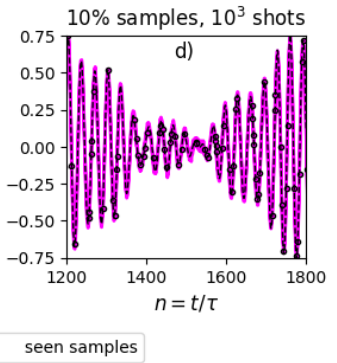
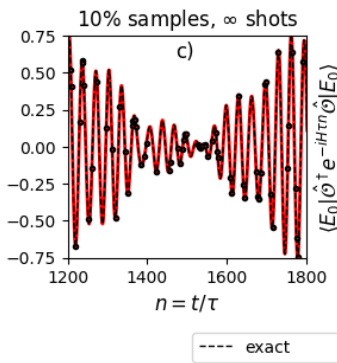
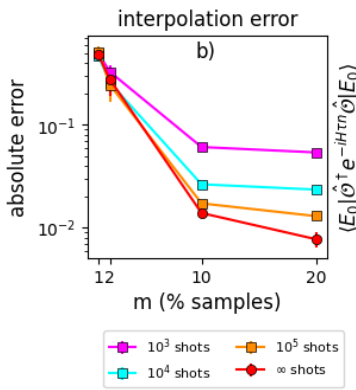
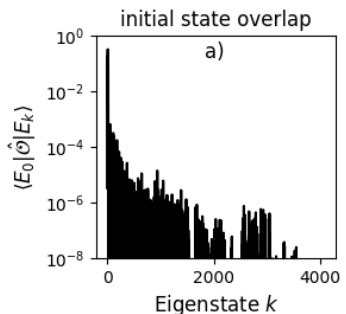
Assuming that we only have access to $m \in \Omega$ samples, and that f is S -sparse in the ψ basis, the optimal solution is given by $f^* = \Psi x^*$, where x^* is the solution of the convex optimization problem

$$\min_{\tilde{x} \in \mathbb{R}^d} \|\tilde{x}\|_1 \text{ subject to } f_k = (\Psi \tilde{x})_k \quad \forall k \in \Omega. \quad (31)$$

d = number of moments

S = number of non-zero components
(sparsity)

// Numerics



DMRG initial state

1. Not good if used with importance sampling.
2. Does not work for extrapolation
3. Always good if you need the whole signal (even with shot noise).

