// Quantum Science Generation – ECT*

Early Fault-Tolerant Quantum Algorithms in Practice:

Application to Ground-State Energy Estimation

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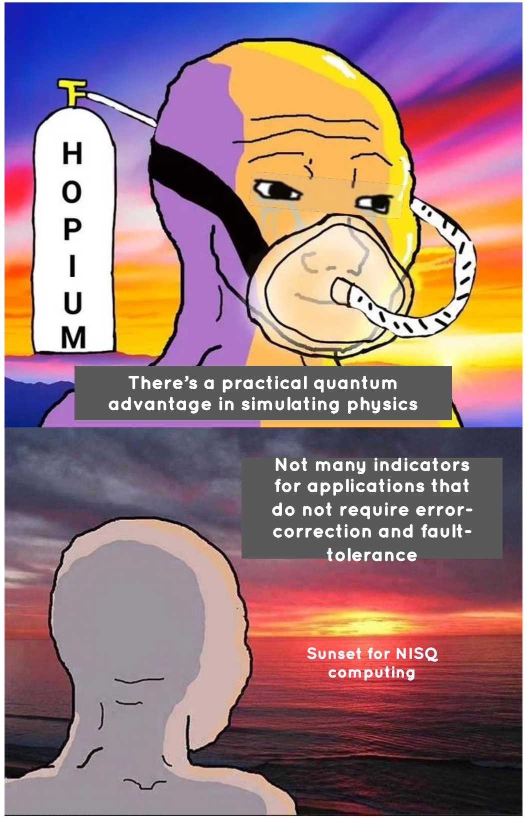
// Motivation

We want to solve a **useful** problem on a quantum computer with an advantage.

Our bet is on **quantum spin models**, but scaling looks a bit scary in terms of precision. Childs, et al. PNAS 115.38 (2018): 9456-9461.

NISQ	Early-FTQC	Fully-FTQC
Variational Algorithms (VQE, QAOA)	ISQ Algorithms (Lin-Tong, Somma, ...)	Phase Estimation (QPE, QETU, filters, ...)
No theoretical arguments for quantum advantage	Optimized Runtime, samples-depth tradeoff, number of qubits	T-gate counts, High-depth Coherent computation
Scaling - ϵ^{-2}	Scaling - ~ $< \epsilon^{-2}$ Prefactor matters!	Scaling - ϵ^{-1}



QETU: Dong, Lin and Tong, PRX Quantum 3, 040305 (2022)

// 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,

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

An Early-FTQC algorithm solving this problems should have following **nice** features:

1. It uses limited (ideally one) or constant ancilla qubits.
2. The circuit depth is $O(\epsilon^{-1})$, i.e., it enjoys Heisenberg scaling.
3. Some degree of robustness against algorithmic errors.

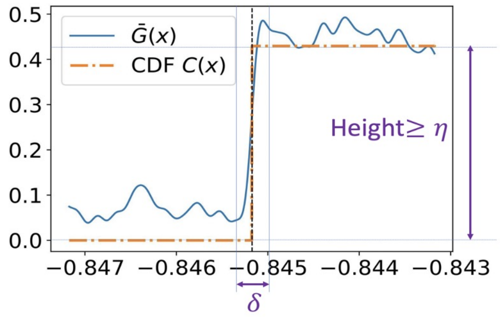
// The Lin-Tong Algorithm

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

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

The LT algorithm does this by approximating the CDF of the spectral measure -

$$p(x) = \sum_k p_k \tilde{\delta}(x - \lambda_k) = \sum_k \mathrm{Tr}[\rho\Pi_k]\tilde{\delta}(x - \lambda_k),$$



Construction:

$$C(x) = p(x) * \Theta(x)$$

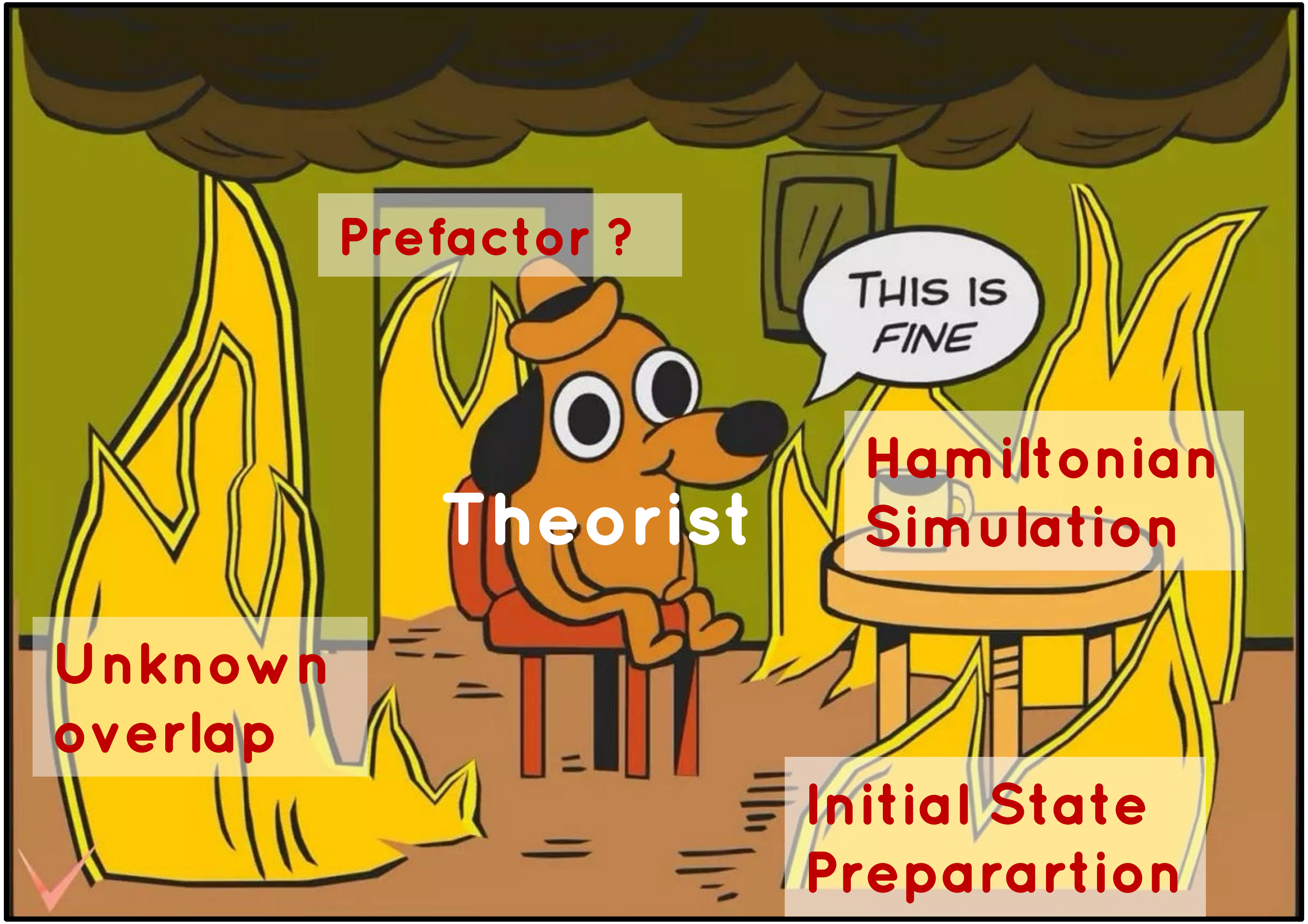
convolution

$$\tilde{C}(x) = \int_{-\pi/2}^{\pi/2} p(y)F(x-y)dy$$
$$= \sum_{|k|\leq D} F_k e^{ikx} \langle\Psi|e^{-i\tau k\mathcal{H}}|\Psi\rangle.$$

Fourier moments computed on the QC with a Hadamard test

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

Lin and Tong PRX Quantum 3, 010318 (2022) , Wan et al. Phys. Rev. Lett. 129, 030503 (2022)


Prefactor ?
THIS IS FINE
Hamiltonian Simulation
Theorist
Unknown overlap
Initial State Preparartion

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// Extinguishing the fire

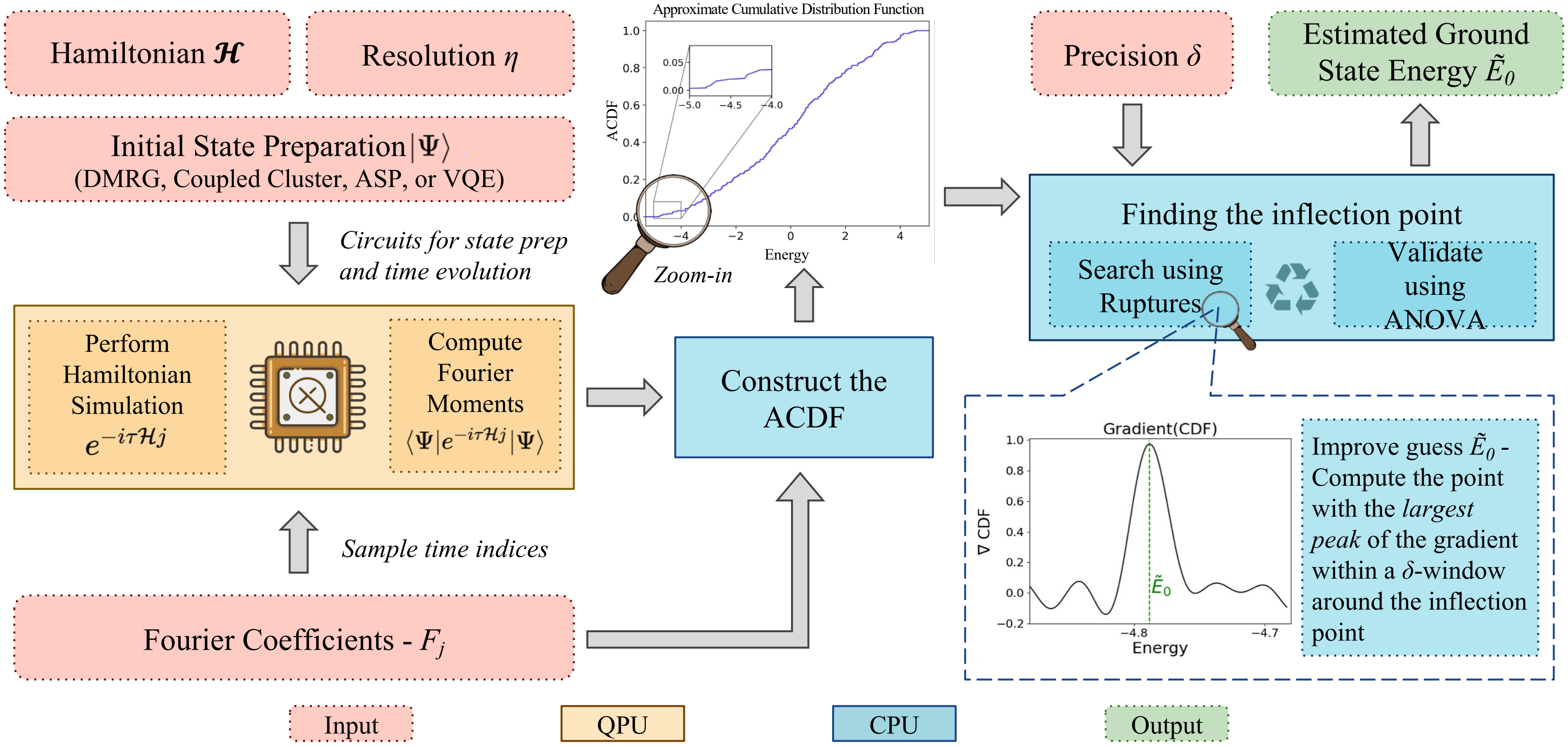
- **Initial State Preparation:** improve from the best you can do classicaly: DMRG, Coupled Cluster, ...
- **Unknown Overlap:** finding the inflection point and looking at the accumulation over the low energy sector.

Accumulation: $$\eta = \sum_{i<m} |\langle E_i|\Psi\rangle|^2,$$

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

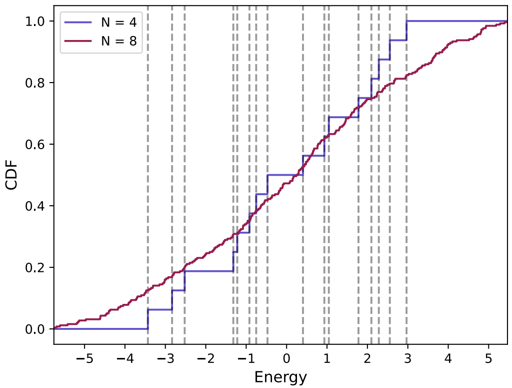
1. no ancilla overhead
2. take advantage of locality
3. often much better than what is guaranteed
4. can scale better than qubitization in some regime

// Our Workflow



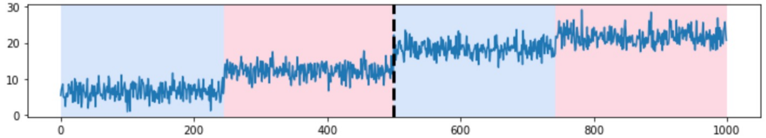
// Key Insights I: Find Inflection

CDF smoothes out with system size (random initial state)



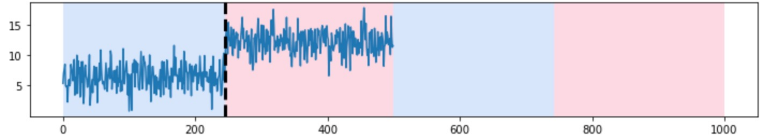
XXZ model

Search a breakpoint



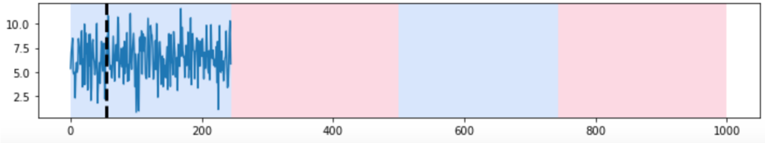
$$\min_{b\in\{1,\dots,n\}} \sum_{t=1}^{b} \|\phi(y_t) - \bar{y}_{1:b}\| + \sum_{t=b+1}^{n} \|\phi(y_t) - \bar{y}_{b+1:n}\|,$$

Improve the breakpoint



Go towards the middle of the jump from the beginning

Validate the breakpoint



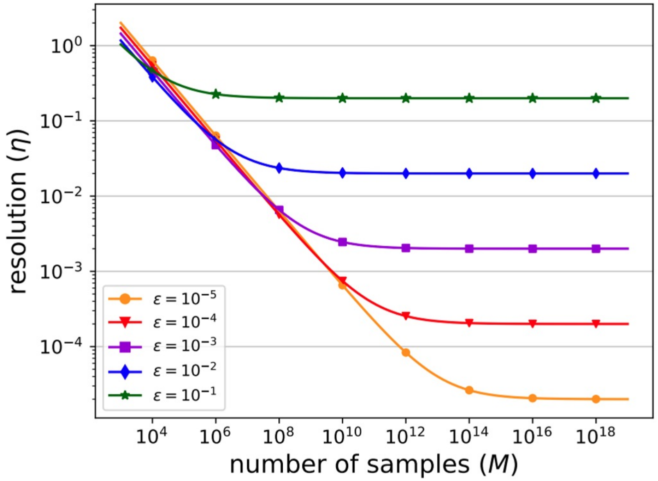
Use ANOVA to test the statistical significance using F-test

Celisse et al, *arXiv:1710.04556*

// Key Insights II: Quantitative Resources

For a given **maximal runtime D** $O(\delta^{-1} \log \delta^{-1}\eta^{-1})$ and accuracy ϵ, the number of samples M required to guarantee the correct result with probability $1 - \vartheta$ is

$$M = \left\lceil 2 \cdot \left[\frac{2.07\pi^{-1}(\log 4D + 1) + 1}{\eta - 2\epsilon} \right]^2 \cdot \left[\log\log\left(\frac{1}{\tau\epsilon}\right) + \log\left(\vartheta^{-1}\right) \right] \right\rceil,$$



To obtain high accuracy, we require more depth (and not only samples).

1. Wan, Berta and Campbell, Phys. Rev. Lett. **129**,030503

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3. **Numerical simulations.**
4. Bonus: application on NISQ devices.

// Numerical Simulations

We consider a fully-connected **Heisenberg model** with random couplings over N spins

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

Why? : universal, gapless, challenging for DMRG.

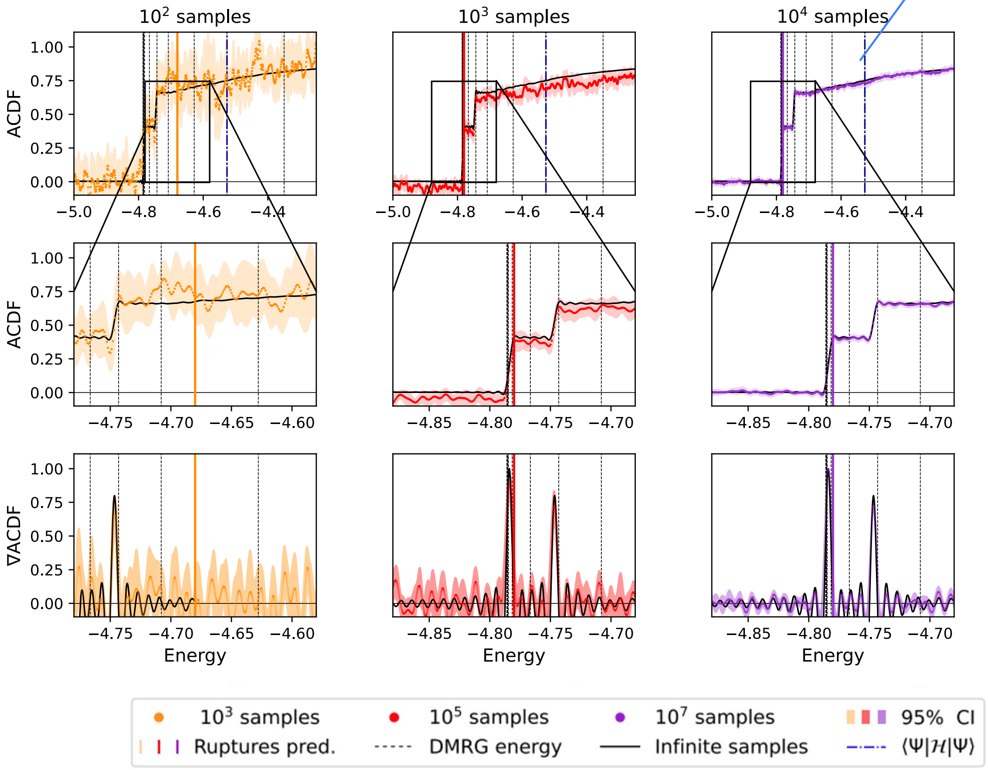
For dynamics we use a **second-order Trotter-Suzuki** with time step $\Delta t = \tau/8$.
The circuit construction is based on SWAP-networks.

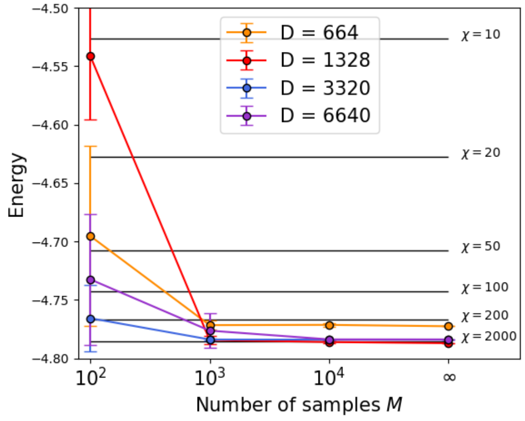
We look at N = 26 spins,
and use initial states prepared via DMRG (with low bond dimension).

Cubitt, Montanaro, and Piddock, Universal quantum Hamiltonians, 115 (38) 9497-9502

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

5% improvment



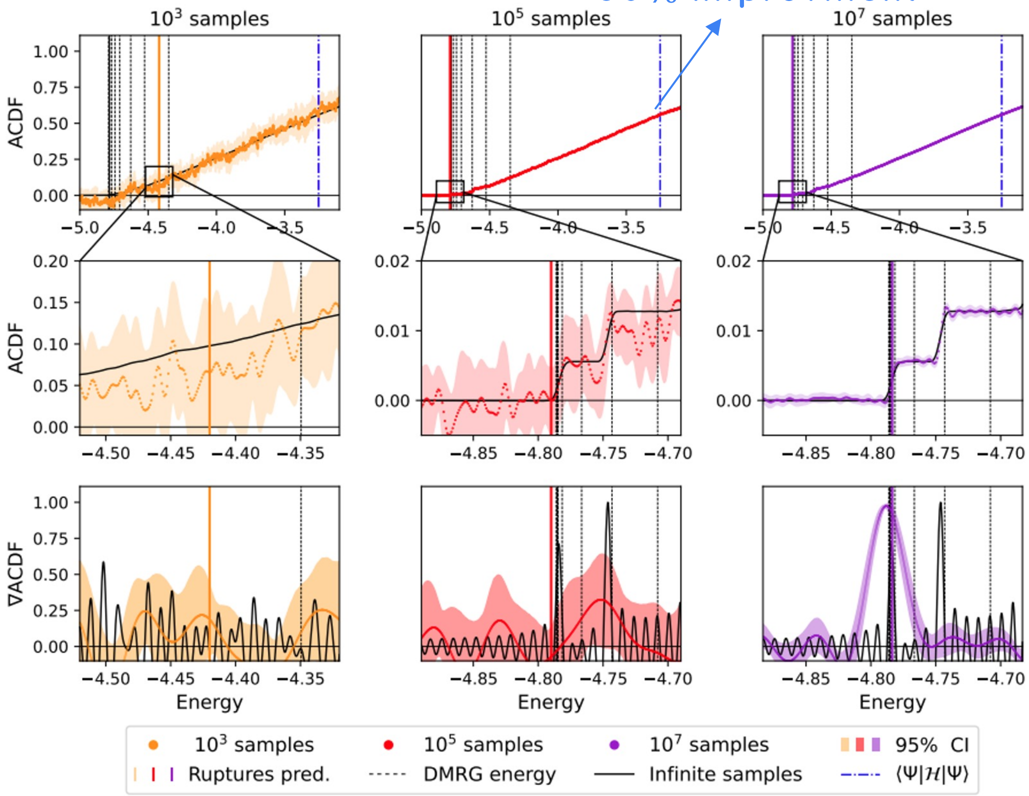


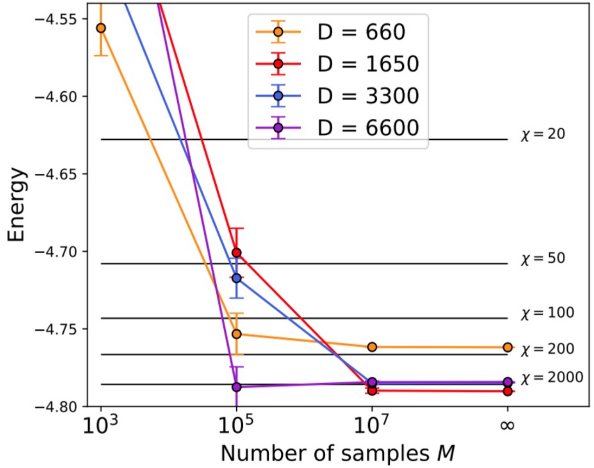
Depth matters most!

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

// Key Insights III: Sparsified DMRG

30% improvment





Fidelity with initial state $p_0 = 7 \times 10^{-3}$

// To Conclude

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. Product formulas are solid candidates for this task.
4. LT algorithms are able to improve on classical solutions, using only limited quantum resources (~10^5 samples).
5. 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.


Simulating
Physics
Classical
Quantum

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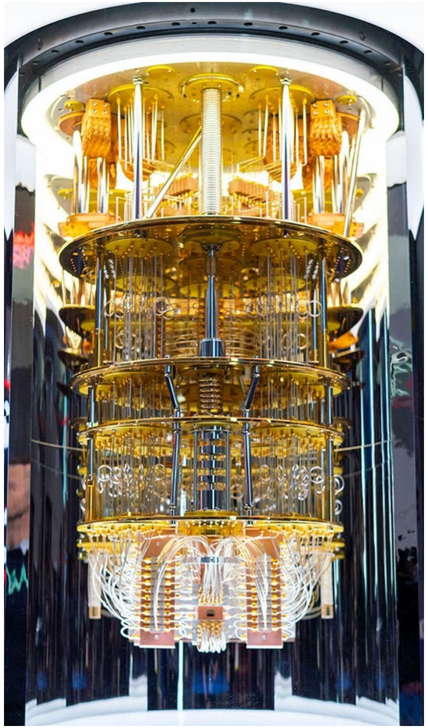
// Bonus: what can we do on NISQ?

- 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 suppresion techniques (twirling, dynamical decoupling, pulse efficient calibration, readout calibration).

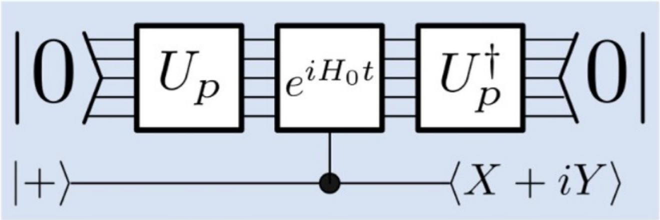


Blunt et al, PRX Quantum 4, 040341 (2023)

// Purified echo verification

Verification

Unprepare the state and verify that it is the zero state



Verification passed → state contributes +/- 1 to the expectation value.

Otherwise → garbage

Purification of the ancilla

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

Pure main component

Noisy components

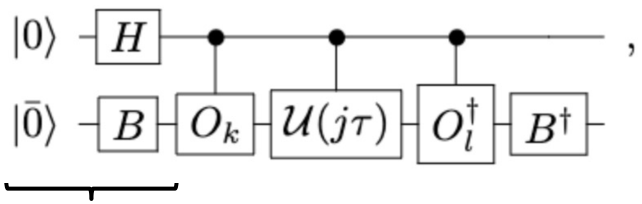
Without noise: the ancilla is pure after post-selection.

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

O'Brien, et al., PRX Quantum 2, 020317 (2021), Huo and Li, Phys. Rev. A 105, 022427 (2022)

// Purified echo verification (details)

Hadamard test



Initial state

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

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

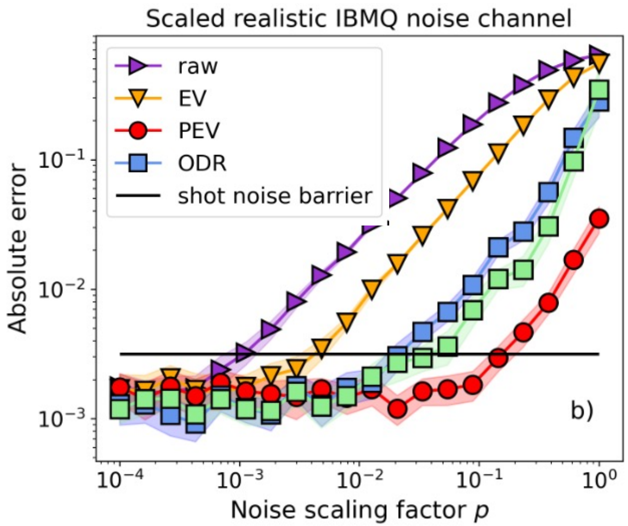
1. We measure the 3 single-qubit Pauli expectation (X,Y and Z) values of the ancilla.

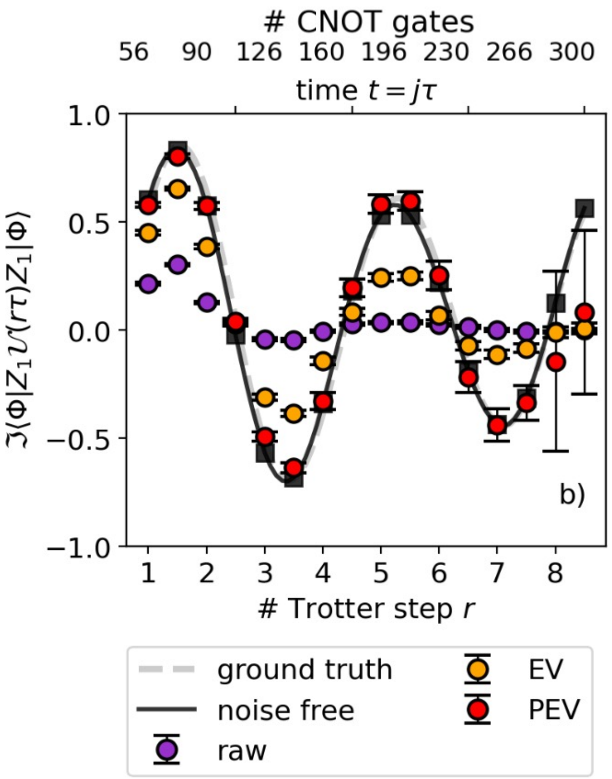
We only care about α, so we can disregard any orthogonal states!

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

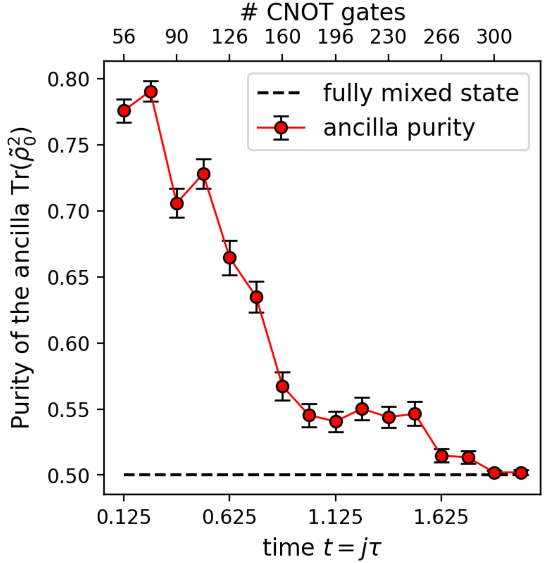
$$\mathrm{Re}\{\alpha\} = \frac{\langle X_a\rangle_0}{1+\langle Z_a\rangle_0}, \quad \mathrm{Im}\{\alpha\} = \frac{\langle Y_a\rangle_0}{1+\langle Z_a\rangle_0}.$$

// Results (IBMQ)





Purity of the ancilla



x100 error reduction

We know the breakpoint

Thank You!
More Questions?

// Team

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arXiv: 2401.13048

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// Key Contributions

- **Relaxation:** finding inflection point and looking at the accumulation over the low-energy sector.

  Accumulation: $$\eta = \sum_{i<m} |\langle E_i|\Psi\rangle|^2,$$

- Gather **quantitative** resource estimates for the LT-algorithm.
- Looking at the **resilience** of the LT-algorithm against the quality of initial state preparation and time evolution.