Workshop on Quantum Chaos, Bernoulli Center

Classical simulation of quantum circuits via Pauli Propagation

October 2nd

Armando Angrisani,
Quantum Information and Computing group

EPFL

"Classically estimating observables of noiseless quantum circuits." arXiv:2409.01706

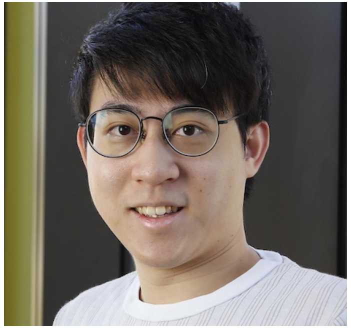
Armando Angrisani
EPFL

Alexander Schmidhuber
MIT

Manuel S. Rudolph
EPFL

Marco Cerezo
LANL

Zoë Holmes
EPFL



Hsin-Yuan Huang
Google, MIT, Caltech

Can chaos enable the classical simulation of quantum systems?

Can chaos enable classical simulation of quantum systems?

it depends on what we mean by ***"simulation"*** *and* ***"chaos"***

Classical simulation of quantum circuits

Given a unitary U and an initial state ρ (typically $|0^n\rangle\langle 0^n|$)

- ➢ Strong simulation: approximate **$U\rho U^\dagger$**
- ➢ Weak simulation:
  - ○ Sample from the **Born distribution** of $U\rho U^\dagger$
  - ○ Given an observable O, estimate **$\mathrm{Tr}[OU\rho U^\dagger]$**

Classical simulation of quantum circuits

Given a unitary U and an initial state ρ (typically $|0^n\rangle\langle 0^n|$)

- Strong simulation: approximate **$U\rho U^\dagger$** — *out of reach for PP*
- Weak simulation:
  - Sample from the **Born distribution** of $U\rho U^\dagger$ — *feasible with PP for **locally scrambling** **noisy** circuits*
  - Given an observable O, estimate **$\mathrm{Tr}[OU\rho U^\dagger]$** — *feasible with PP for **locally scrambling** circuits*

<u>PP = Pauli Propagation, a family of simulation algorithms</u>

An extreme case: Haar-random state

- Sampling from the Born distribution of a Haar-random state is “classically hard”
  Still true for the output of random circuits

An extreme case: Haar-random state

➢ Sampling from the Born distribution of a Haar-random state is “classically hard”
Still true for the output of random circuits
⇒ Experimental demonstration of quantum supremacy

Article | Published: 23 October 2019

Quantum supremacy using a programmable superconducting processor

Frank Arute, Kunal Arya, Ryan Babbush, Dave Bacon, Joseph C. Bardin, Rami Barends, Rupak Biswas, Sergio Boixo, Fernando G. S. L. Brandao, David A. Buell, Brian Burkett, Yu Chen, Zijun Chen, Ben Chiaro, Roberto Collins, William Courtney, Andrew Dunsworth, Edward Farhi, Brooks Foxen, Austin Fowler, Craig Gidney, Marissa Giustina, Rob Graff, Keith Guerin, ... John M. Martinis + Show authors

An extreme case: Haar-random state

➢ Sampling from the Born distribution of a Haar-random state is hard
Still true for the output of random circuits
⇒ Experimental demonstration of quantum supremacy

Article | Published: 23 October 2019

Quantum supremacy using a programmable superconducting processor

Frank Arute, Kunal Arya, Ryan Babbush, Dave Bacon, Joseph C. Bardin, Rami Barends, Rupak Biswas, Sergio Boixo, Fernando G. S. L. Brandao, David A. Buell, Brian Burkett, Yu Chen, Zijun Chen, Ben Chiaro, Roberto Collins, William Courtney, Andrew Dunsworth, Edward Farhi, Brooks Foxen, Austin Fowler, Craig Gidney, Marissa Giustina, Rob Graff, Keith Guerin, ... John M. Martinis + Show authors

➢ Any expectation value will be close to zero!

An extreme case: “highly random” states

- Sampling from the Born distribution of a Haar-random state is hard
  Still true for the output of random circuits
  ⇒ Experimental demonstration of quantum supremacy

Article | Published: 23 October 2019

Quantum supremacy using a programmable superconducting proce

Frank Arute, Kunal Arya, Ryan Babbush, Dav
Sergio Boixo, Fernando G. S. L. Brandao, Da
Roberto Collins, William Courtney, Andrew D
Gidney, Marissa Giustina, Rob Graff, Keith Guerin, ... John M. Martinis
+ Show authors

NEWS | PHYSICS

Ordinary computers can beat Google's quantum computer after all

Superfast algorithm put crimp in 2019 claim that Google's machine had achieved “quantum supremacy”

2 AUG 2022 · 5:05 PM · BY ADRIAN CHO

- Any expectation value will be close to zero!

Chaos and scrambling

- Quantum chaos "scrambles" local information quickly across an entire system (e.g. black holes)

- The time evolution of the system is a **pseudo-Haar-random** process

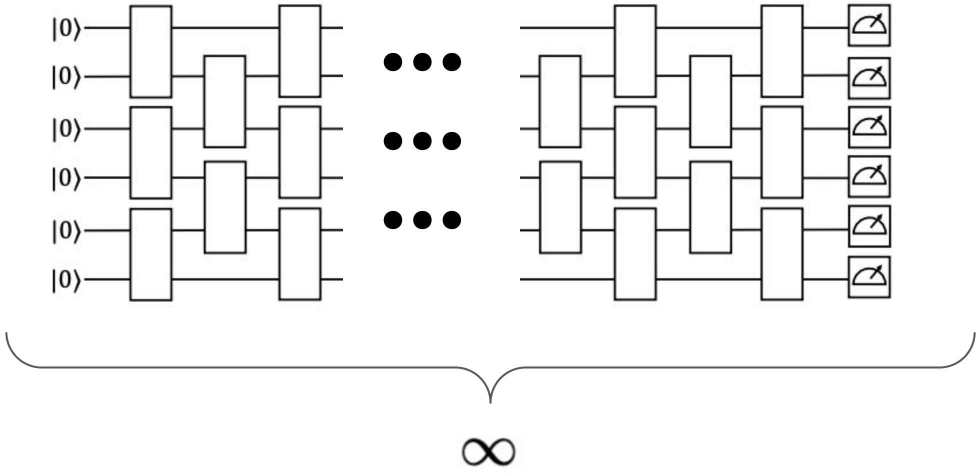
$$W(t) = e^{iHt} W e^{-iHt}$$

(H chaotic Hamiltonian, W local operator)

Roberts, Daniel A., and Beni Yoshida. "Chaos and complexity by design." Journal of High Energy Physics 2017.4 (2017): 1-64.

Chaos and Random Quantum Circuits

Infinite-depth random circuits are Haar-random



Probing chaos

H Hamiltonian

V, W local operators

$$W(t) = e^{iHt} W e^{-iHt}$$

$$W(t)^\dagger V^\dagger W(t) V$$

(group commutator)

Probing chaos

H chaotic Hamiltonian

V, W local operators

$$W(t) = e^{iHt} W e^{-iHt}$$

$$W(t)^{\dagger} V^{\dagger} W(t) V$$

→ $\approx I$ — *non-chaotic*

→ global, random operator — *chaotic*

Probing chaos

H chaotic Hamiltonian

V, W local operators

$$W(t) = e^{iHt} W e^{-iHt}$$

$$W(t)^\dagger V^\dagger W(t) V \longrightarrow \approx I$$

non-chaotic

Probing chaos with Out-of-Time-Order 4-point functions

H chaotic Hamiltonian

V, W local operators

$$W(t) = e^{iHt} W e^{-iHt}$$

$$\mathrm{Tr}\left[W(t)^{\dagger} V^{\dagger} W(t) V \rho_H\right]$$

→ ≈ 1 *non-chaotic*

→ ≈ 0 *chaotic*

$$\rho_H = \frac{e^{-\beta H}}{\mathrm{Tr}[e^{-\beta H}]}$$

Probing chaos with Out-of-Time-Order 4-point functions

H chaotic Hamiltonian

V, W local operators

$$W(t) = e^{iHt} W e^{-iHt}$$

$$\mathrm{Tr}\left[W(t)^\dagger V^\dagger W(t) V \rho_H\right]$$

≈ 1 *non-chaotic*

what's in the middle?

≈ 0 *chaotic*

$$\rho_H = \frac{e^{-\beta H}}{\mathrm{Tr}[e^{-\beta H}]}$$

OTO functions and 2-designs

$$\mathrm{Tr}\big[W(t)^\dagger V^\dagger W\ \ (t) V \rho_H\big]$$

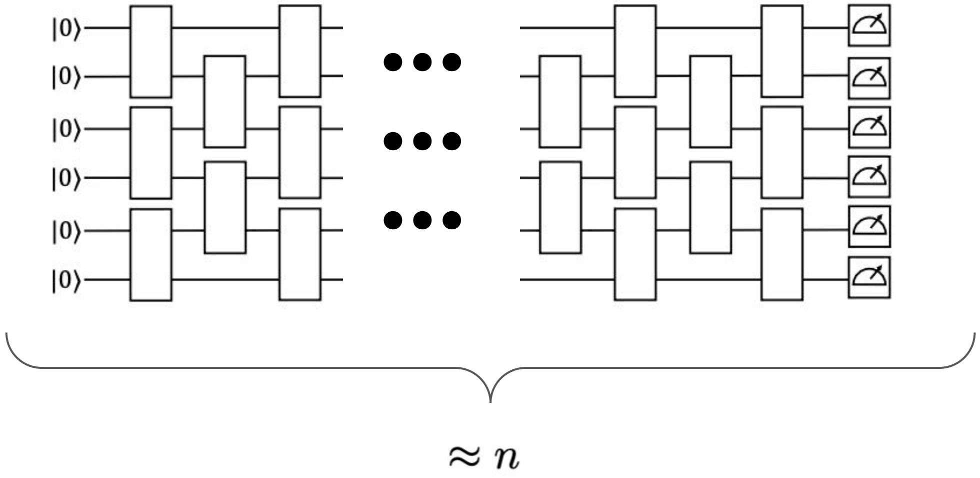
The OTO function contains only second moments of the chaotic Hamiltonian

⇒ We can approximate the chaotic evolution with a unitary 2-design

$$\mathbb{E}_{U\sim\nu} U^{\dagger\otimes 2} O U^{\otimes 2} \approx \mathbb{E}_{U\sim\nu_{\mathrm{Haar}}} U^{\dagger\otimes 2} O U^{\otimes 2}$$

Chaos and Random Quantum Circuits, II

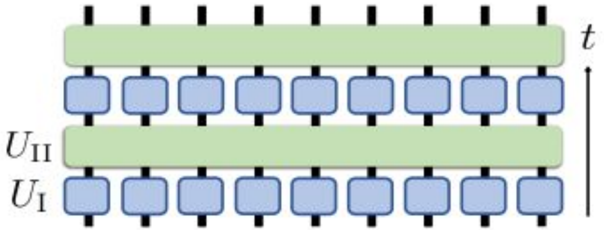
Linear-depth random circuits are approximate 2-designs

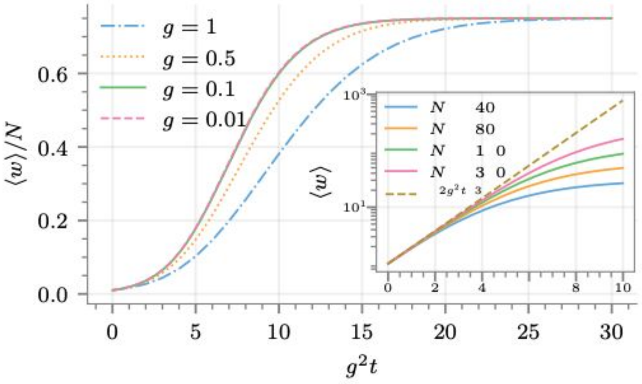


Chaos and Random Quantum Circuits, III

Random single qubit gates suffices for highly chaotic behaviour

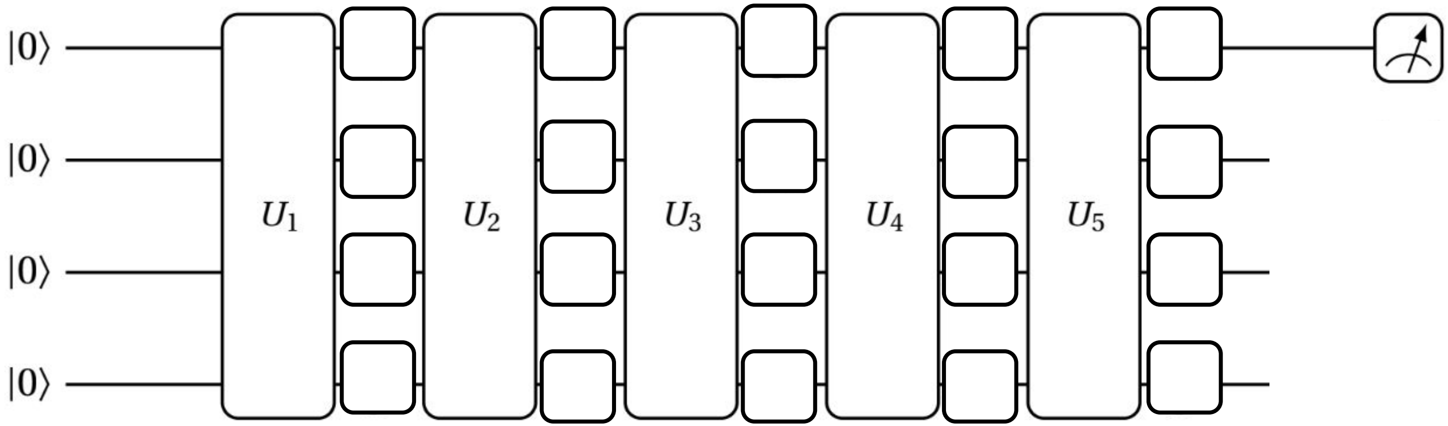
$$U_{\mathrm{I}} = \prod_{i=1}^{N} U_{H,i}, \qquad U_{\mathrm{II}} = e^{-i \frac{g}{2\sqrt{N}} \sum_{i<j} Z_i Z_j}$$





Belyansky, Ron, et al. "Minimal model for fast scrambling." Physical review letters 125.13 (2020): 130601.

Locally scrambling circuit



- All single-qubit gates sampled i.i.d. from local 2-designs
- Arbitrary entangling layers U_i's

The problem

Given a locally scrambling quantum U,

can we approximate $Tr[OU\rho U^{\dagger}]$ with a classical computer?

The problem

Given a locally scrambling circuit U,
can we approximate $\mathrm{Tr}[OU\rho U^\dagger]$ with a classical computer?

Yes!
It takes poly(n) time, for any constant precision

Motivations

- ➢ Many physical processes are approximately locally scrambling
- ➢ Variational quantum circuits are often initialized at random
- ➢ Understand why the Pauli Propagation algorithm works so well in practice
  – This is a “simple” model in which we can prove things

The Heisenberg picture

$\mathrm{Tr}[OU\rho U^\dagger] = \mathrm{Tr}[U^\dagger OU\rho]$

$\rightarrow$ Compute (approximately) $U^\dagger OU$ and project it onto ρ

The Heisenberg picture

$\mathrm{Tr}[OU\rho U^\dagger] = \mathrm{Tr}[U^\dagger OU\rho]$

$\rightarrow$ Compute (approximately) $U^\dagger OU$ and project it onto ρ

$$O = \frac{1}{2^n} \sum_{P \in \{I,X,Y,Z\}^{\otimes n}} \mathrm{Tr}[OP]P$$

$$U = U_L U_{L-1} \dots U_1$$

$$\rho = |0^n\rangle\langle 0^n|$$

$$\begin{cases} U_j^\dagger P U_j = \sum_{P \in \{I,X,Y,Z\}^{\otimes n}} a_P P \\ \text{with } \sum_{P \in \{I,X,Y,Z\}^{\otimes n}} a_P^2 = 1 \end{cases}$$

The Heisenberg picture

Tr[OUρU†] = Tr[U†OUρ]

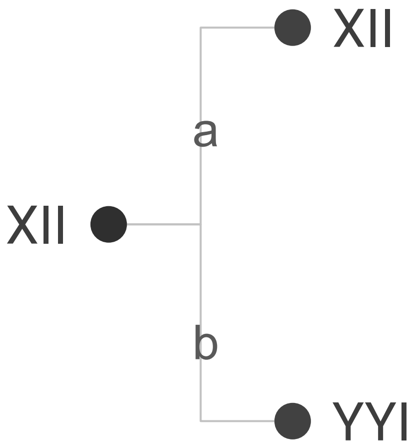
→ Compute (approximately) U†OU and project it onto ρ

$$O = \frac{1}{2^n} \sum_{P \in \{I,X,Y,Z\}^{\otimes n}} \mathrm{Tr}[OP]P$$

$$U = U_L U_{L-1} \dots U_1$$

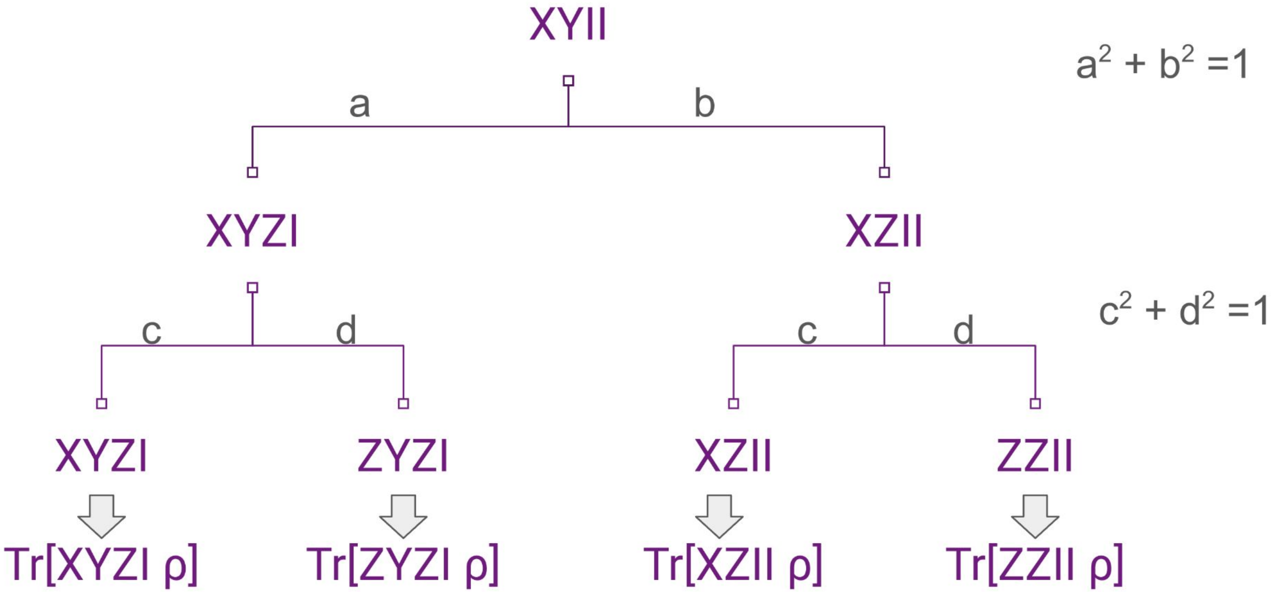
$$\rho = |0^n\rangle\langle 0^n|$$

$$\begin{cases} U_j^\dagger P U_j = \sum_{P \in \{I,X,Y,Z\}^{\otimes n}} a_P P \\ \text{with } \sum_{P \in \{I,X,Y,Z\}^{\otimes n}} a_P^2 = 1 \end{cases}$$



$$U^\dagger(XII)U = a\,XII + b\,YYI$$

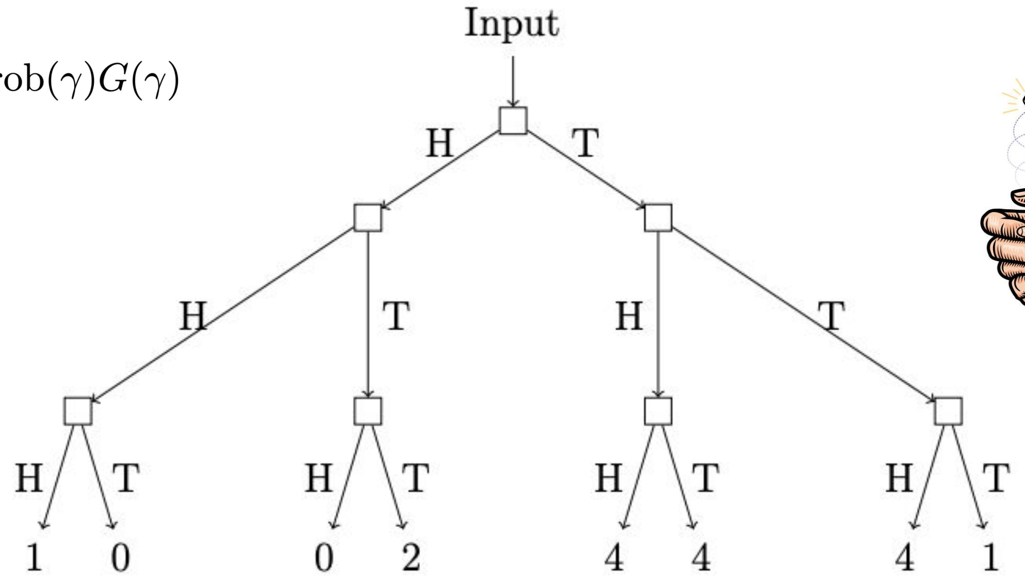
Tree-like representation of Quantum Computation



$$F(XYII) = \sum_{\gamma \in \text{paths}} \Phi(\gamma)\, \mathrm{Tr}[P_\gamma \rho]$$

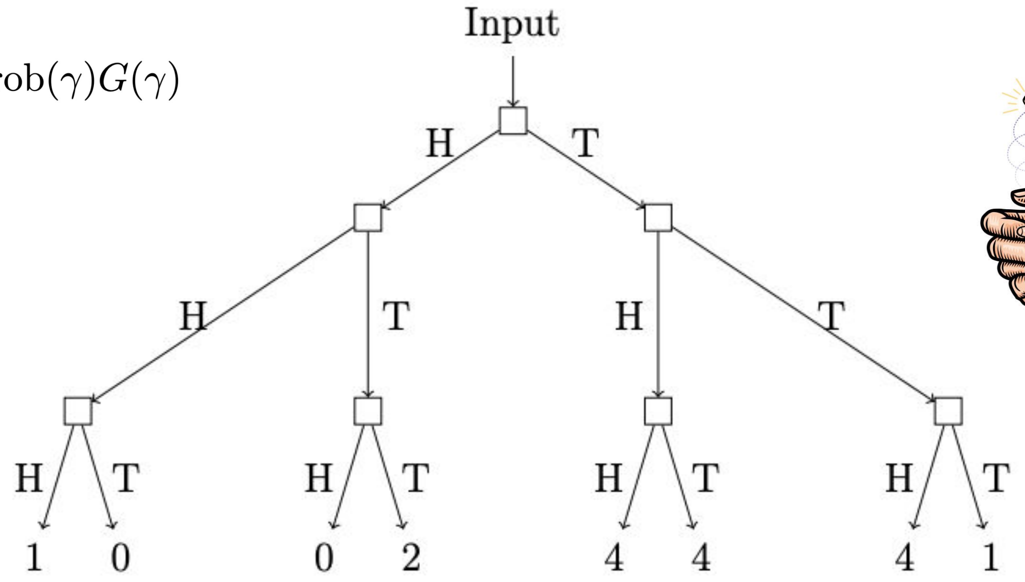
A step back: classical Randomized Computation

$$F(\text{Input}) = \sum_{\gamma \in \text{paths}} \text{Prob}(\gamma) G(\gamma)$$



A step back: classical Randomized Computation

$$F(\text{Input}) = \sum_{\gamma \in \text{paths}} \text{Prob}(\gamma) G(\gamma)$$



Expected values efficiently computable by Monte-Carlo sampling paths!

- ➢ Computing exactly or Monte Carlo sampling Pauli paths is classically intractable
- ➢ Can we find a sub-tree which carries most of the useful information?

Are all Pauli paths created equal?

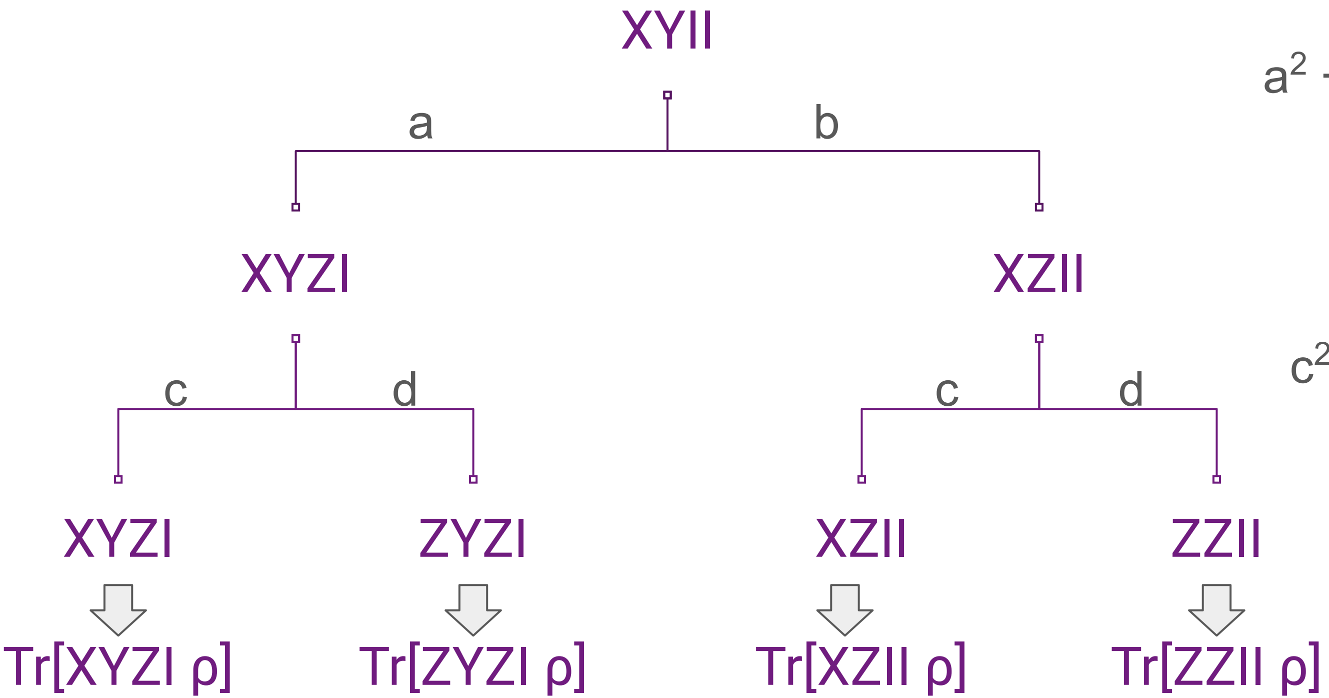
Pauli-weight: number of non-identity terms in a Pauli operator

ex. weight(IXYIZ) = 3
weight(IIIII) = 0

Paths with high-weight Paulis can be truncated if

- the circuit is noisy
- the circuit is locally scrambling,
  <u>and we want to estimate expectation values</u>

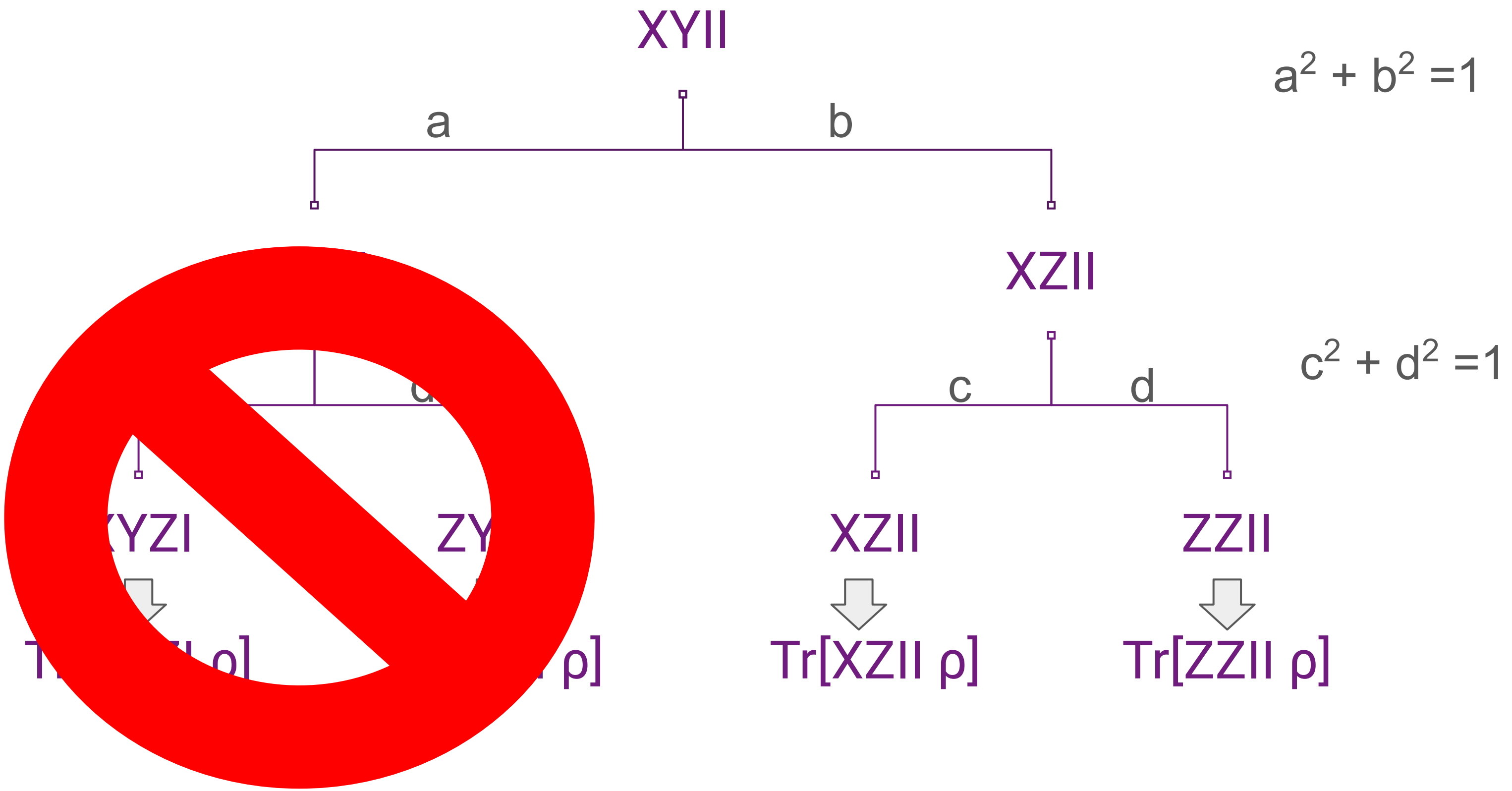
Tree-like representation of Quantum Computation



$a^2 + b^2 = 1$

$c^2 + d^2 = 1$

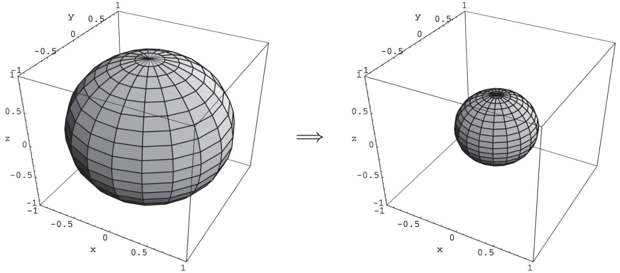
Tree-like representation of Quantum Computation



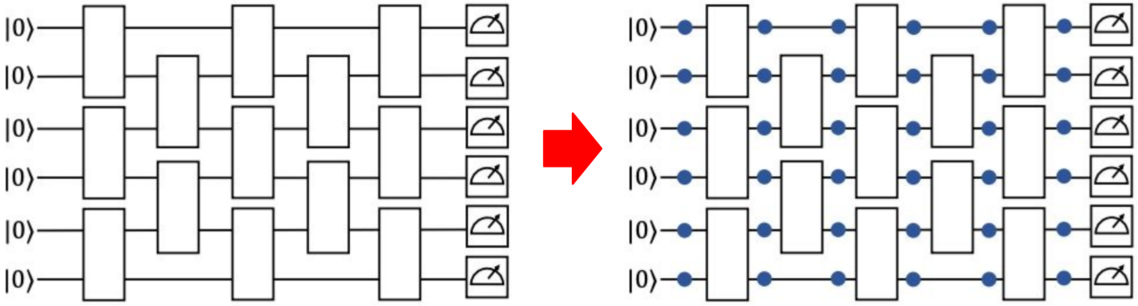
The noisy case

- Single-qubit depolarizing noise

$$\mathcal{D}_p(\rho) = p\frac{I}{2} + (1-p)\rho$$



- Noisy circuits

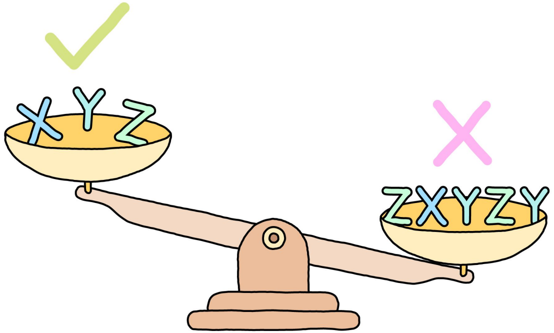


The noisy case

$$\mathcal{D}_p^{\otimes n}(P) = (1-p)^{\mathrm{weight}(P)} P$$

$$\implies \left|\mathrm{Tr}\left[\mathcal{D}_p^{\otimes n}(P)\rho\right]\right| \leq (1-p)^{\mathrm{weight}(P)}$$

Paths containing **high-weight** Paulis are **exponentially** suppressed!



The noisy case

A polynomial-time classical algorithm for noisy random circuit sampling

Dorit Aharonov* Xun Gao† Zeph Landau‡ Yunchao Liu§ Umesh Vazirani¶

'22

Classical simulations of noisy variational quantum circuits

Enrico Fontana[1,2,3,*] Manuel S. Rudolph[4], Ross Duncan[2], Ivan Rungger[3], and Cristina Cîrstoiu[2]

'23

A polynomial-time classical algorithm for noisy quantum circuits

Thomas Schuster,[1,*] Chao Yin,[2,*] Xun Gao,[2,3] and Norman Y. Yao[4]

'24

The noisy case

A polynomial-time classical algorithm for noisy random circuit sampling

Dorit Aharonov* Xun Gao† Zeph Landau‡ Yunchao Liu§ Umesh Vazirani¶

‘22

locally scrambling circuits

Classical simulations of noisy variational quantum circuits

Enrico Fontana[1,2,3,*] Manuel S. Rudolph[4], Ross Duncan[2], Ivan Rungger[3], and Cristina Cîrstoiu[2]

‘23

parametrized circuits

A polynomial-time classical algorithm for noisy quantum circuits

Thomas Schuster,[1,*] Chao Yin,[2,*] Xun Gao,[2,3] and Norman Y. Yao[4]

‘24

arbitrary circuits with input sampled from a 1-design

The noisy case

A polynomial-time classical algori
sampli

Dorit Aharonov* Xun Gao† Zeph Landa

pling circuits

Classical simulations of noisy v

Enrico Fontana[1,2,3,*] Manuel S. Rudolph[4], Ross D

circuits

A polynomial-time classical algorith

Thomas Schuster,[1,*] Chao Yin,[2,*] Xun

uits with input
a 1-design

However, the same simulation algorithm works well on “typical” noiseless circuits

Classical surrogate simulation of quantum systems with LOWESA

Manuel S. Rudolph,[1,2,*] Enrico Fontana,[3,4,5,6] Zoë Holmes,[1] and Lukasz Cincio[2]

simulates

Evidence for the utility of quantum computing before fault tolerance

Youngseok Kim, Andrew Eddins, Sajant Anand, Ken Xuan Wei, Ewout van den Berg, Sami Rosenblatt, Hasan Nayfeh, Yantao Wu, Michael Zaletel, Kristan Temme & Abhinav Kandala

Nature **618**, 500–505 (2023)

Quantum Convolutional Neural Networks are (Effectively) Classically Simulable

Pablo Bermejo,[1,2,3] Paolo Braccia,[4] Manuel S. Rudolph,[5] Zoë Holmes,[5] Lukasz Cincio,[4] and M. Cerezo[1,*] However, th[...] works well

c

Classical surrog[...]vith LOWESA

Manuel S. Rudolp[...] Lukasz Cincio[2]

simula

quantum computing before

nd, Ken Xuan Wei, Ewout van den Berg, Sami
aletel, Kristan Temme & Abhinav Kandala

Quantum Convolution[...]Classically Simulable

Pablo Bermejo,[1,2,3] Paolo Br[...] Cincio,[4] and M. Cerezo[1,*]

2-designs in the Heisenberg picture

Given a unitary U sampled from a 2-design, we have for any non-identity P

$$\mathbb{E}_U U^{\dagger\otimes 2} P^{\otimes 2} U^{\otimes 2} = \frac{1}{4^n - 1} \sum_{P \neq I} P^{\otimes 2}$$

The single-qubit case

$$\mathbb{E}_U U^{\otimes 2\dagger} X^{\otimes 2} U^{\otimes 2} = \frac{1}{3}(X^{\otimes 2} + Y^{\otimes 2} + Z^{\otimes 2})$$

Scrambling vs Expectation values

- Without randomness

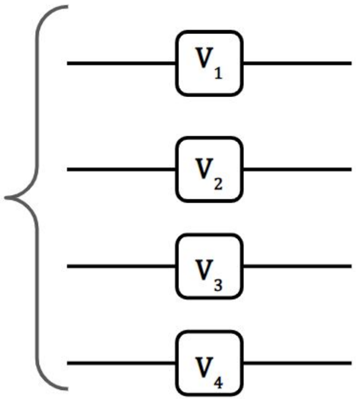
$$\mathrm{Tr}[X\rho] \in [-1, 1]$$

- With randomness

$$\begin{aligned}\mathbb{E}_U \, \mathrm{Tr}\big[XU\rho U^\dagger\big]^2 &= \frac{1}{3}\left(\mathrm{Tr}[X\rho]^2 + \mathrm{Tr}[Y\rho]^2 + \mathrm{Tr}[Z\rho]^2\right) \\ &= \frac{2}{3} \cdot \underbrace{\frac{1}{2}\left(\mathrm{Tr}[X\rho]^2 + \mathrm{Tr}[Y\rho]^2 + \mathrm{Tr}[Z\rho]^2\right)}_{< \mathrm{Tr}[\rho^2] \leq 1} \leq \frac{2}{3}\end{aligned}$$

Locally scrambling layer

$$U = V_1 \otimes V_2 \otimes V_3 \otimes V_4$$



$$\mathbb{E}_U \operatorname{Tr}\left[P U \rho U^\dagger\right]^2 \leq \left(\frac{2}{3}\right)^{\mathrm{weight}(P)}$$

Huang, Hsin-Yuan, Sitan Chen, and John Preskill. "Learning to predict arbitrary quantum processes." PRX Quantum 4.4 (2023): 040337.

$$\mathbb{E}_U \operatorname{Tr}\left[PU\rho U^\dagger\right]^2 \leq \left(\frac{2}{3}\right)^{\text{weight}(P)}$$

$$\left|\operatorname{Tr}\left[\mathcal{D}_p^{\otimes n}(P)\rho\right]\right| \leq (1-p)^{\text{weight}(P)}$$

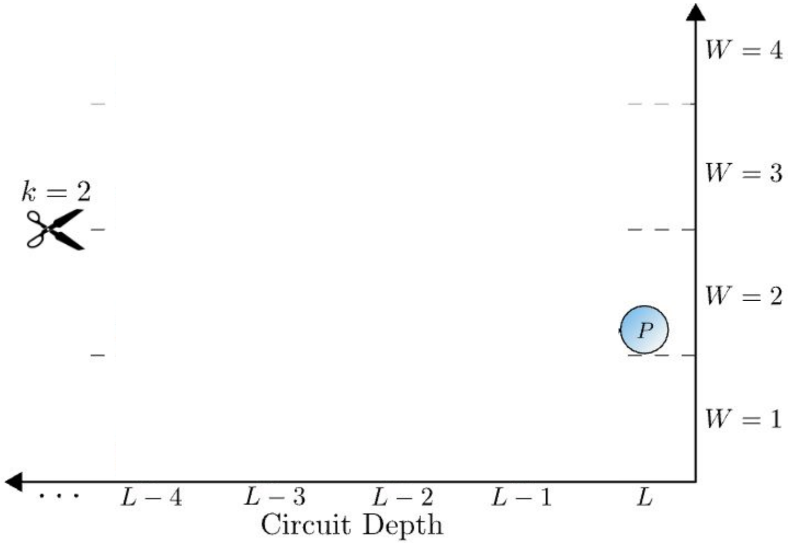
A "weight-truncated" observable

$$O = \sum_P a_P P$$

$$O^{(k)} = \sum_{\substack{P: \\ \text{weight}(P)<k}} a_P P$$

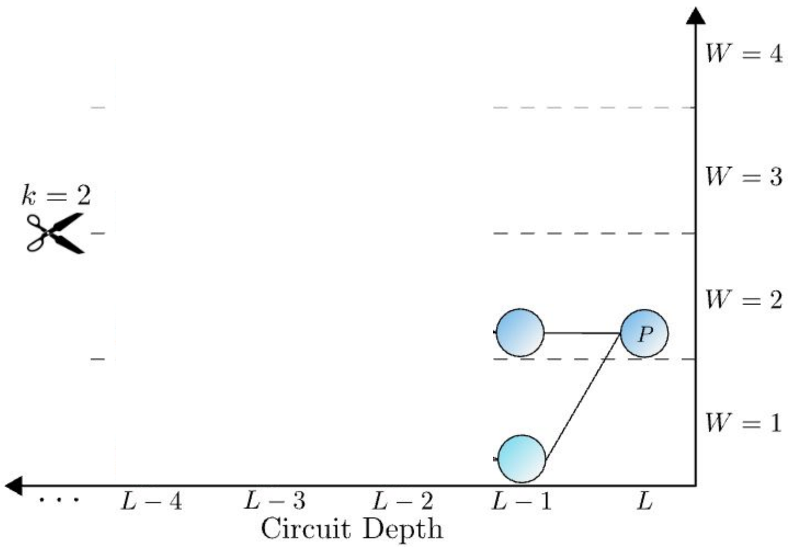
$$\mathbb{E}_U \operatorname{Tr}\left[\left(O - O^{(k)}\right) U \rho U^\dagger\right]^2 \leq \left(\frac{2}{3}\right)^k \|O\|$$

“Weight-truncated” Pauli Propagation



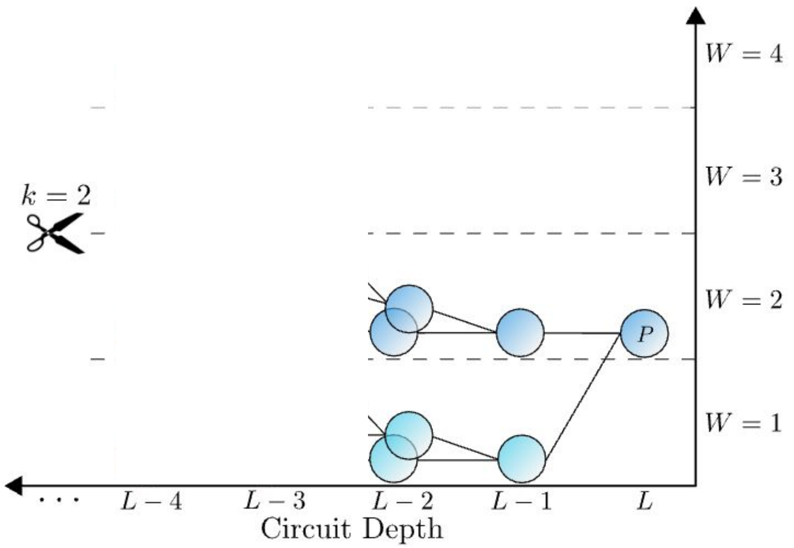
All Paulis with weight > k are truncated

“Weight-truncated” Pauli Propagation



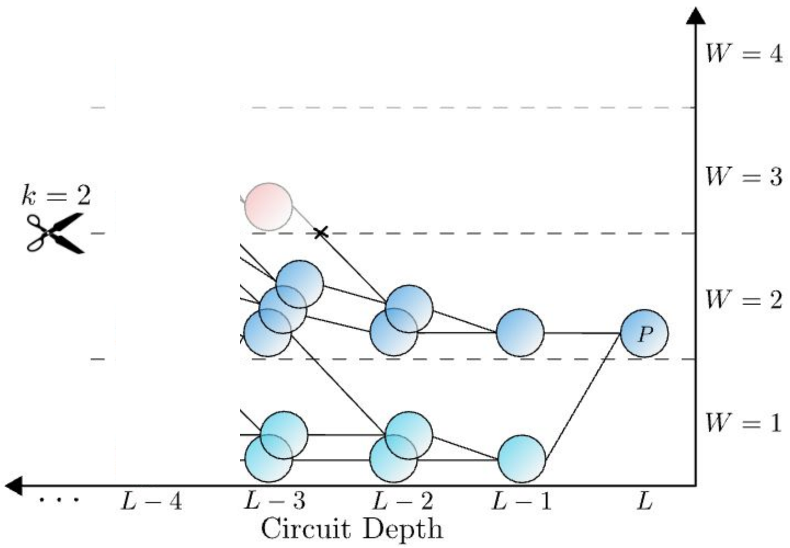
All Paulis with weight > k are truncated

"Weight-truncated" Pauli Propagation



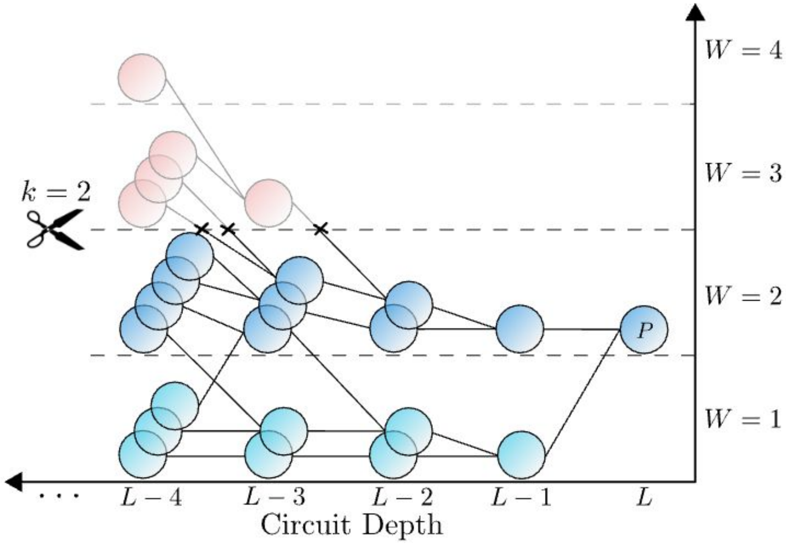
All Paulis with weight > k are truncated

"Weight-truncated" Pauli Propagation



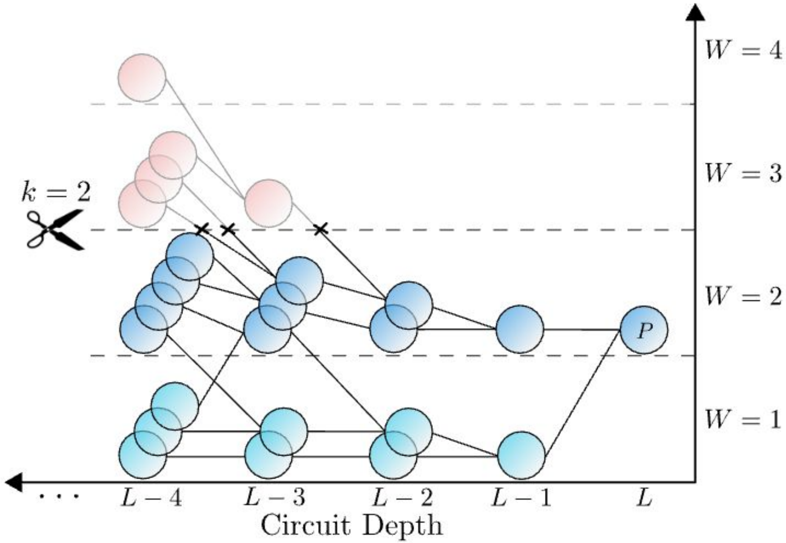
All Paulis with weight > k are truncated

"Weight-truncated" Pauli Propagation



All Paulis with weight > k are truncated

“Weight-truncated” Pauli Propagation



$$\mathbb{E}_U \operatorname{Tr}\left[\left(U^\dagger O U - (U^\dagger O U)^{(\mathrm{apx})}\right)\rho\right]^2 \leq \left(\frac{2}{3}\right)^k \|O\|$$

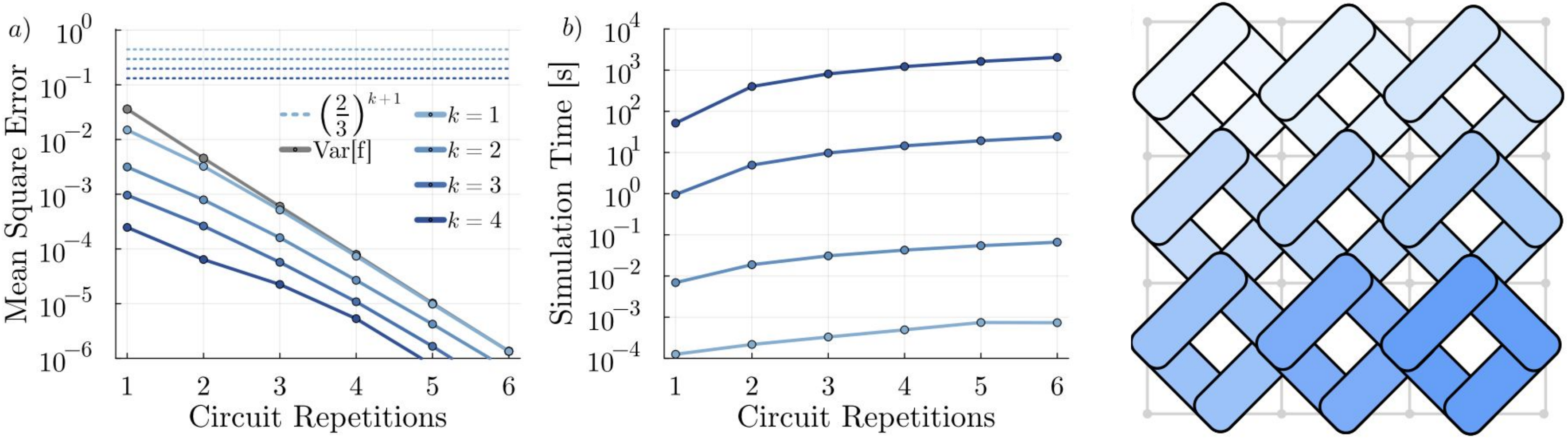
“Weight-truncated” Pauli Propagation

- ➢ Error bound depends only on k

- ➢ Polynomial complexity for constant error

- ➢ Easy to “certify” numerically
  → Experiments demonstrate faster convergence

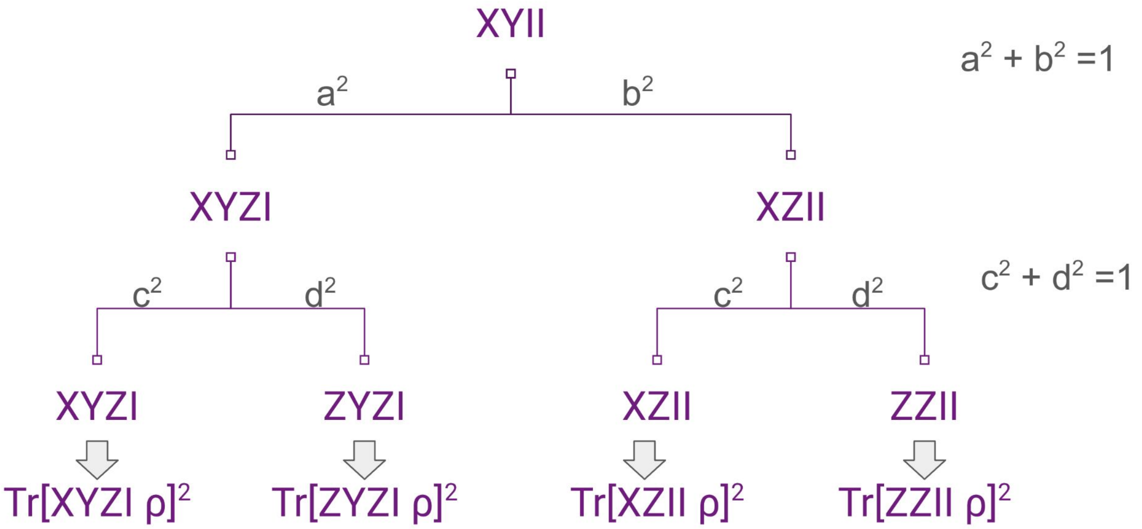
2D Staircase Topology on 64 qubits



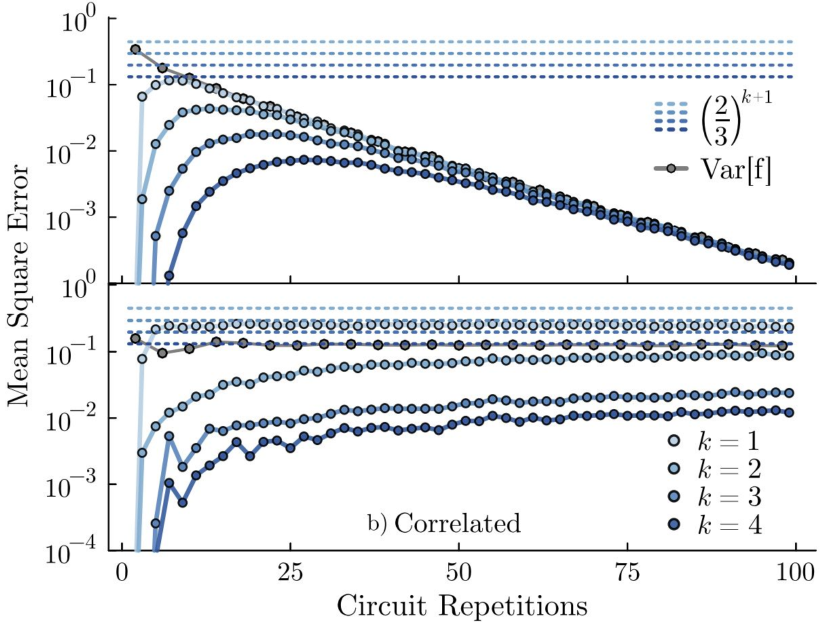
Zhang, Hao-Kai, Shuo Liu, and Shi-Xin Zhang. "Absence of barren plateaus in finite local-depth circuits with long-range entanglement." Physical Review Letters 132.15 (2024): 150603.

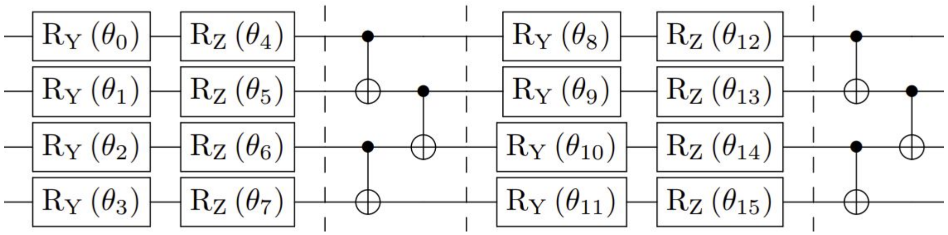
Numerical certification: intuition

- ➢ The average error depends only on the squared amplitudes a^2, b^2, c^2, d^2 ...
- ➢ Then we can MC sample the Pauli tree!



Experiments beyond our bounds





Classical Simulation via Pauli Propagation

- ➢ Naturally harnesses noise and scrambling
- ➢ Not natively hindered by entanglement or circuit connectivity

Caveats

- ➢ Theoretical guarantees only in certain settings (uncorrelated gates)
- ➢ Not suitable for sampling from noiseless circuits

Related works on quantum chaos

Low-weight truncations strategies have been developed independently by several research communities!

- Von Keyserlingk, Curt, Frank Pollmann, and Tibor Rakovszky. **"Operator backflow and the classical simulation of quantum transport."** Physical Review B 105.24 (2022): 245101.
- Rakovszky, Tibor, C. W. Von Keyserlingk, and Frank Pollmann. **"Dissipation-assisted operator evolution method for capturing hydrodynamic transport."** Physical Review B 105.7 (2022): 075131.
- Ramos-Marimón, Carlos, Stefano Carignano, and Luca Tagliacozzo. **"Pauli weight requirement of the matrix elements in time-evolved local operators: dependence beyond the equilibration temperature."** arXiv:2409.13603 (2024).

Related works on quantum chaos

Low-weight truncations strategies have been developed independently by several research communities!

- Von Keyserlingk, Curt, Frank Pollmann, and Tibor Rakovszky. **"Operator backflow and the classical simulation of quantum transport."** Physical Review B 105.24 (2022): 245101.

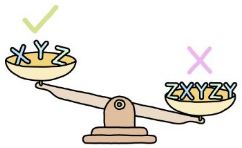
- Rakovszky, Tibor, C. W. Von Keyserlingk, and Frank Pollmann. **"Dissipation-assisted operator evolution method for capturing hydrodynamic transport."** Physical Review B 105.7 (2022): 075131.

- Ramos-Marimón, Carlos, Stefano Carignano, and Luca Tagliacozzo. **"Pauli weight requirement of the matrix elements in time-evolved local operators: dependence beyond the equilibration temperature."** arXiv:2409.13603 (2024).

We need a unified framework!

arXiv

Thanks!
Questions?



Demo

Classically estimating expectation values from...