

A randomized quantum algorithm for statistical phase estimation

arXiv:2110.12071 (with Kianna Wan and Earl Campbell)





Part of: Quantum algorithms for learning the energy spectrum of quantum systems

Earl Campbell (Part I) & Mario Berta (Part II)

AWS Center for Quantum Computing

Problem: Ground state energy estimation

- Given n -qubit Hamiltonian

$$H := \sum_{l=1}^L \alpha_l P_l \text{ with } P_l \text{ } n\text{-qubit Paulis}$$

and one-norm $\lambda := \sum_{l=1}^L |\alpha_l|$, together with efficiently preparable n -qubit ansatz state ρ with overlap

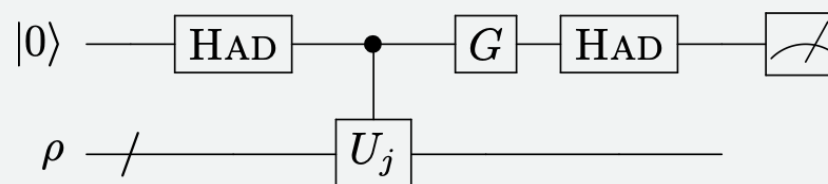
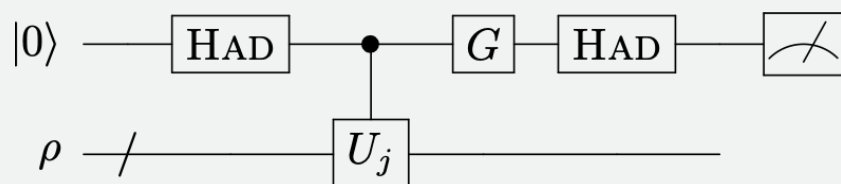
$$\langle \phi_0 | \rho | \phi_0 \rangle \geq \eta > 0$$

for ground state $|\phi_0\rangle\langle\phi_0|$ with energy E_0

- **Goal: Compute estimate \tilde{E}_0 with precision $|\tilde{E}_0 - E_0| \leq \Delta$**

Goals for early fault-tolerance scheme

1. Minimize number of qubits needed – only one ancilla



2. Independent of the number L of Pauli terms in H – instead, depending one-norm $\lambda \leq L$
3. Trade-off gate versus sample complexity
4. Decrease error by solely taking more samples

Main result



Algorithm ground state energy estimation

- Output \tilde{E}_0 with $|\tilde{E}_0 - E_0| \leq \Delta$ with probability $1 - \xi$ by employing

$$C_{sample} = \tilde{O}(\eta^{-2}) \quad [= o(\eta^{-2} \log^2(\lambda \Delta^{-1} \log(\eta^{-1})) \log(\xi^{-1} \log(\lambda \Delta^{-1})))]$$

quantum circuits on $n + 1$ qubits, each using one copy of ρ and

$$C_{gate} = \tilde{O}(\lambda^2 \Delta^{-2}) \quad [= o(\lambda^2 \Delta^{-2} \log^2(\eta^{-1}))]$$

single-qubit Pauli rotations $\exp(i\theta P_l)$

- Plus: Clifford gates – generated by CNOT, H, and S (Paulis)

Complexity ground state energy estimation

- n qubit Hamiltonian, $n + 1$ qubits with quantum complexities independent of L :

$$C_{gate} = \tilde{O}(\lambda^2 \Delta^{-2}) \text{ for } C_{sample} = \tilde{O}(\eta^{-2})$$

- Randomized algorithm with classical pre- and post-processing
- Comparison state-of-the-art qubitization based approach:

$$\text{gate complexity } \tilde{O}(\sqrt{L}\lambda\Delta^{-1}) \text{ for } \tilde{O}(\sqrt{L}) \text{ qubits} \rightarrow \text{total } \tilde{O}(L\lambda\Delta^{-1})$$

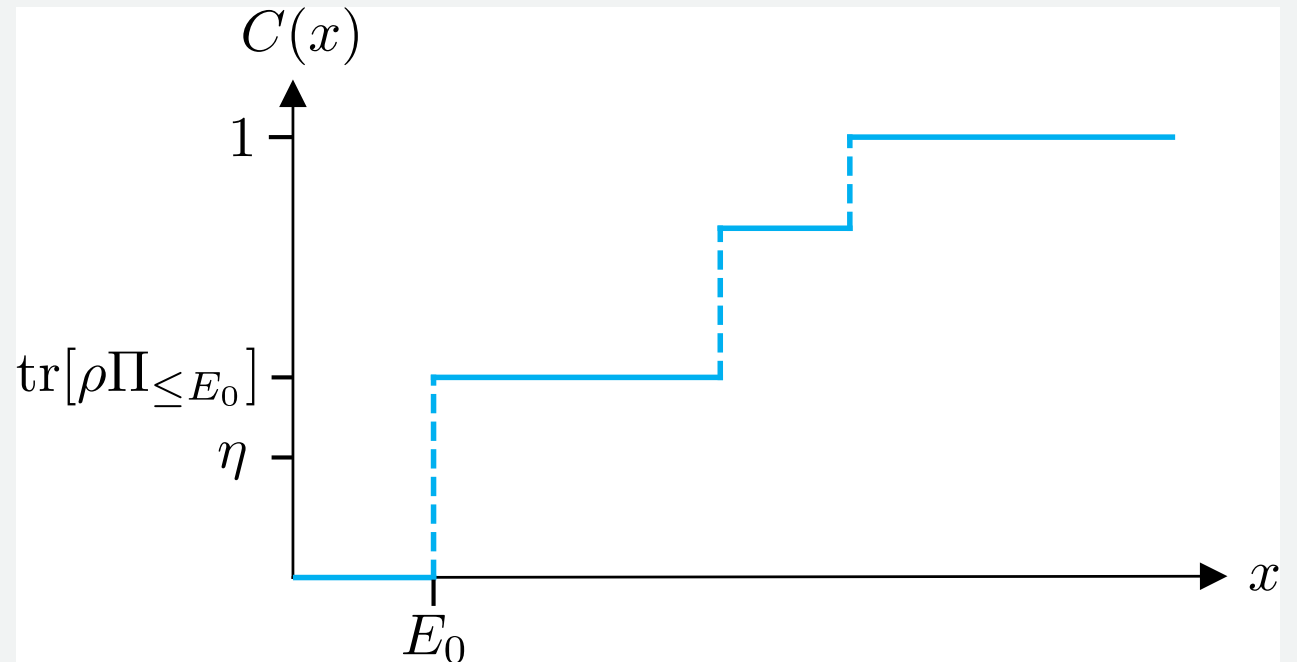
[Lee et al., PRX Quantum (2021)]

Basic idea

- Cumulative distribution function (CDF) relative to ρ :

$$C(x) := \text{Tr}[\rho \Pi_{\leq x}]$$

- Evaluate $C(x)$ from quantum routine?
- Eigenvalue thresholding
- Give ground state energy estimate \tilde{E}_0 via binary search



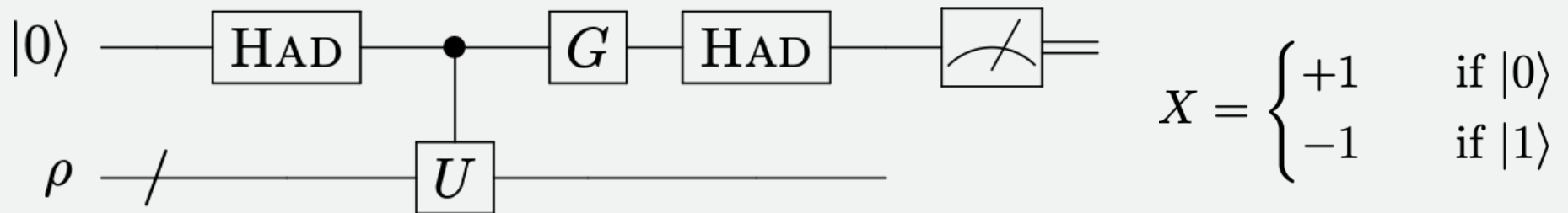
[Lin & Tong, arxiv:2102.112340 (2021)]
[Martyn et al., arxiv:2105.02859 (2021)]

Quantum routine to evaluate CDF



Workhorse A: Hadamard test

- Input: n -qubit state ρ together with n -qubit unitary U
- Circuit:



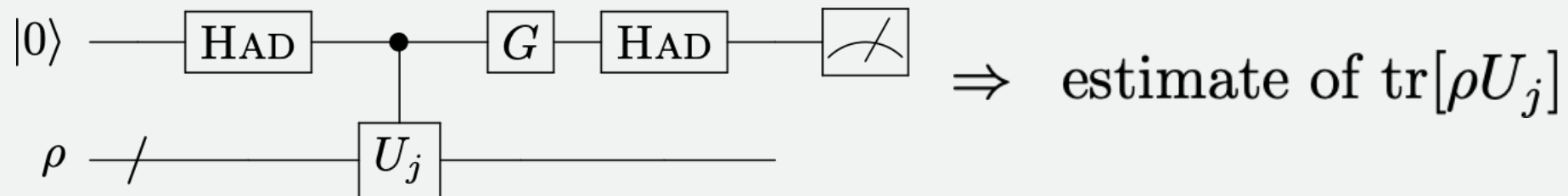
- Output: **unbiased estimate of $\text{Tr}[\rho U]$** from

$$G = I \quad \Rightarrow \quad \mathbb{E}[X] = \text{Re}(\text{tr}[\rho U])$$

$$G = S^\dagger \quad \Rightarrow \quad \mathbb{E}[X] = \text{Im}(\text{tr}[\rho U])$$

Workhorse B: Importance sampling

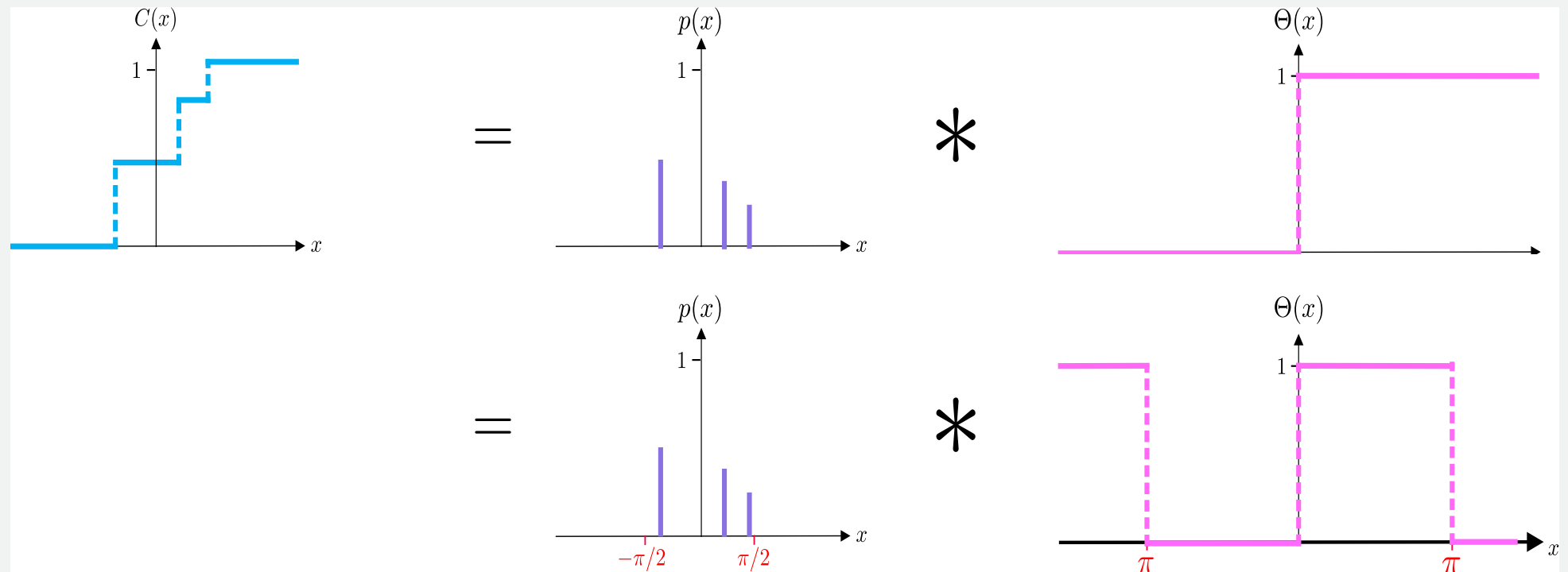
- Estimate linear combination $\sum_j a_j \text{Tr}[\rho U_j]$ for unitaries U_j with $a_j > 0$ and normalization $A := \sum_j a_j$
- Sample j with probability $a_j \cdot A^{-1}$ and perform Hadamard test on (ρ, U_j) :



- Take average of samples, number of required is $\lceil A^2 \sigma^{-2} \rceil$ for variance $\sigma > 0$
- Expected gate complexity becomes $A^{-1} \cdot \sum_j a_j \text{COST}(C - U_j)$

Towards quantum implementation of CDF

- Normalize Hamiltonian with $c \cdot \|H\|_\infty \leq c \cdot \lambda$ to put spectrum in $\left[-\frac{\pi}{2}, +\frac{\pi}{2}\right]$
- CDF $C(x) \equiv \text{Tr}[\rho \Pi_{\leq x}] = (\Theta * p)(x)$ from convolution with Heaviside $\Theta(x)$:



CDF via Fourier series

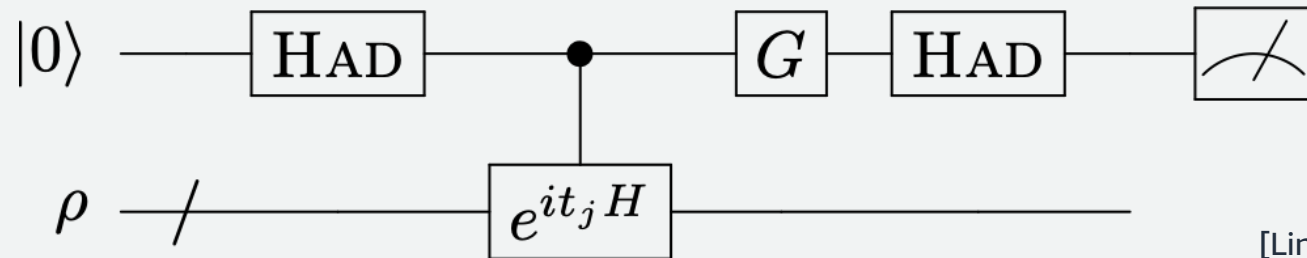
- Replace Heaviside $\Theta(x)$ by finite Fourier series $F(x) := \sum_{j \in \mathcal{S}} \hat{F}_j e^{ijx}$

- Approximate CDF:

$$C(x) \approx (p * F)(x) = \sum_{j \in \mathcal{S}} \hat{F}_j e^{ijx} \cdot \text{Tr}[\rho e^{it_j H}]$$

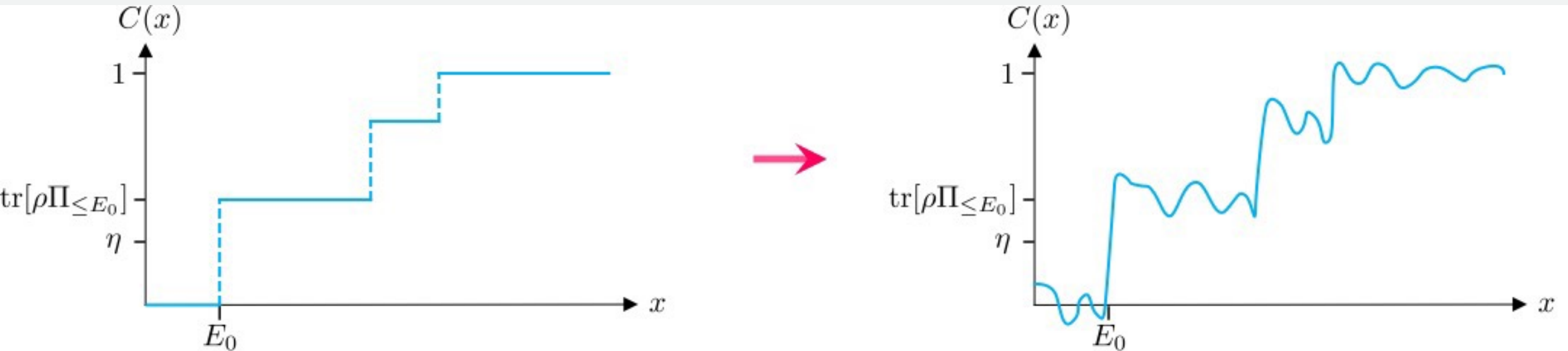
with runtimes $t_j = j \times \text{normalization}$

- Hadamard test + importance sampling + Hamiltonian simulation:



[Lin & Tong, arxiv:2102.112340 (2021)]

Fourier series lemma (Heaviside function)

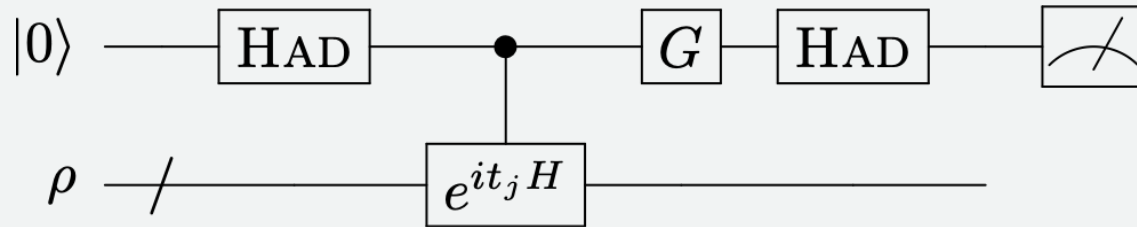


- Improved Fourier series approximation of Heaviside function
- Technical contribution:

gate complexity for precision $\Delta > 0$ from $O(\Delta^{-2} \log^2(\Delta^{-1}))$ to $O(\Delta^{-2})$

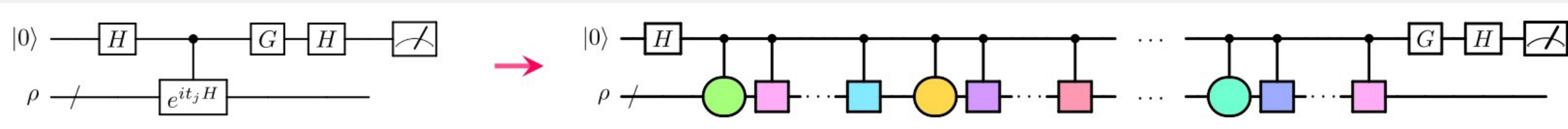
[Lin & Tong, arxiv:2102.112340 (2021)]

Hadamard test on Fourier series



$$C(x) \approx \sum_{j \in S} \hat{F}_j e^{ijx} \cdot \text{Tr}[\rho e^{it_j H}]$$

- Implement Hamiltonian simulation unitary $U_j = e^{it_j H}$ for $H = \sum_{l=1}^L \alpha_l P_l$
- Independent of L ? Technical contribution:



novel random compiler lemma (Hamiltonian simulation)

Versus previous random compiler:
[Campbell, PRL (2019)]

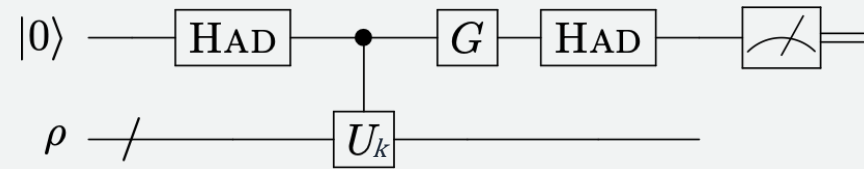
Random compiler lemma (Hamiltonian simulation)

- For e^{itH} with $H = \sum_{l=1}^L \alpha_l P_l$, we give linear combination of unitaries (LCU)

$$e^{itH} = \sum_k b_k U_k \text{ such that:}$$

$$I. \quad \mu(r) := \sum_k b_k \leq \exp(t^2 r^{-1})$$

$$II. \quad \text{COST}(C - U_k) = r \text{ controlled single qubit Pauli rotations } \forall k$$



- Gate complexity r versus sample complexity $\exp(t^2 r^{-1})$

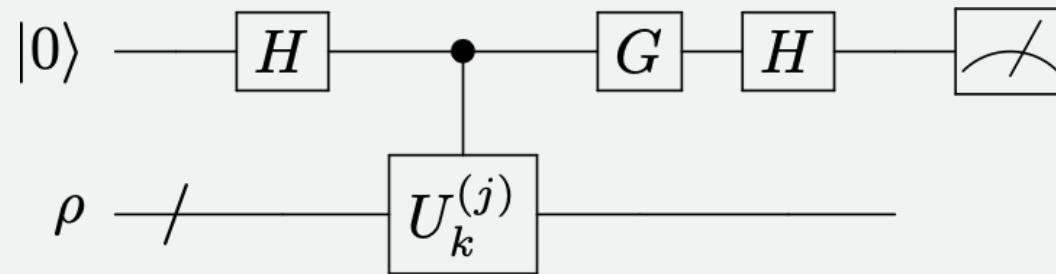
Versus previous LCU methods:
[Berry et al., PRL (2015)]

- Example: $r = 2t^2 \rightarrow \mu \leq \sqrt{e}$ and $\text{COST}(C - U_k) = 2t^2$

- Use this on: $C(x) \approx \sum_{j \in S} \hat{F}_j e^{ijx} \cdot \text{Tr}[\rho e^{it_j H}]$

Random compiler for CDF

- CDF $C(x) \approx \sum_j \hat{F}_j e^{ijx} \cdot \text{Tr}[\rho e^{it_j H}]$ becomes $C(x) \approx \sum_j \sum_k \hat{F}_j e^{ijx} b_k^{(j)} \text{Tr}[\rho U_k^{(j)}]$



- $e^{it_j H} = \sum_k b_k^{(j)} U_k^{(j)}$ decomposition for runtime vector $\vec{r} = (r_j)_{j \in \mathbb{N}^{|S|}}$ as:

- I. $\mu_j := \mu_j(r) := \sum_k b_k^{(j)} \leq \exp(t_j^2 r_j^{-1})$

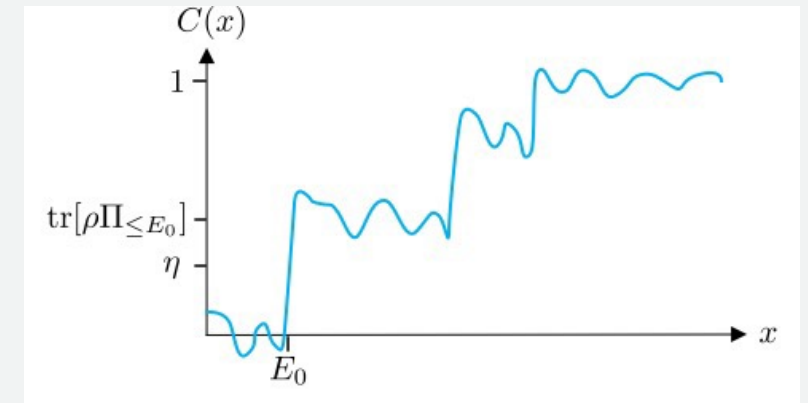
- II. $\text{COST}(C - U_k^{(j)}) = r_j$

Putting things together

- CDF decomposition $C(x) \approx \sum_j \sum_k \hat{F}_j e^{ijx} b_k^{(j)} \text{Tr} [\rho U_k^{(j)}]$
- $C_{gate} = \left(\sum_{i \in S} |\hat{F}_i| \mu_i \right)^{-1} \cdot \left(\sum_{j \in S} |\hat{F}_j| \mu_j r_j \right)$
- $C_{sample} \propto \left(\sum_{j \in S} |\hat{F}_j| \mu_j \right)^2$
- As $\mu_j \leq e^{t_j^2 r_j^{-1}}$ choosing $r_j = 2t_j^2 \forall j$ gives $\mu_j \leq \sqrt{e}$:

$$C_{gate} \propto \left(\sum_{i \in S} |\hat{F}_i| \right)^{-1} \left(\sum_{j \in S} |\hat{F}_j| j^2 \right) \rightarrow C_{gate} = \tilde{O}(\lambda^2 \Delta^{-2})$$

$$C_{sample} \propto \left(\sum_{j \in S} |\hat{F}_j| \right)^2 \rightarrow C_{sample} = \tilde{O}(\eta^{-2})$$

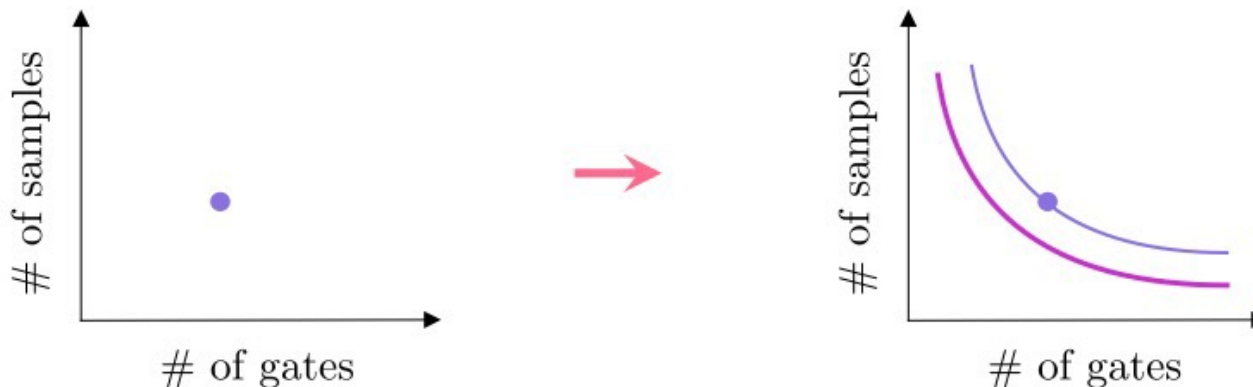


Example systems



Finite size numerical analysis

- Asymptotic complexity from fixed runtime vector \vec{r} with $r_j = 2t_j^2 \forall j \in S$
- Optimize \vec{r} to minimize C_{gate} , C_{sample} , or $C_{gate} \cdot C_{sample}$ for different settings?
- High-dimensional optimization problem, technical contribution: approximate dimension reduction that allows for **efficient classical pre-processing**
- Leads to flexible resource trade-offs:

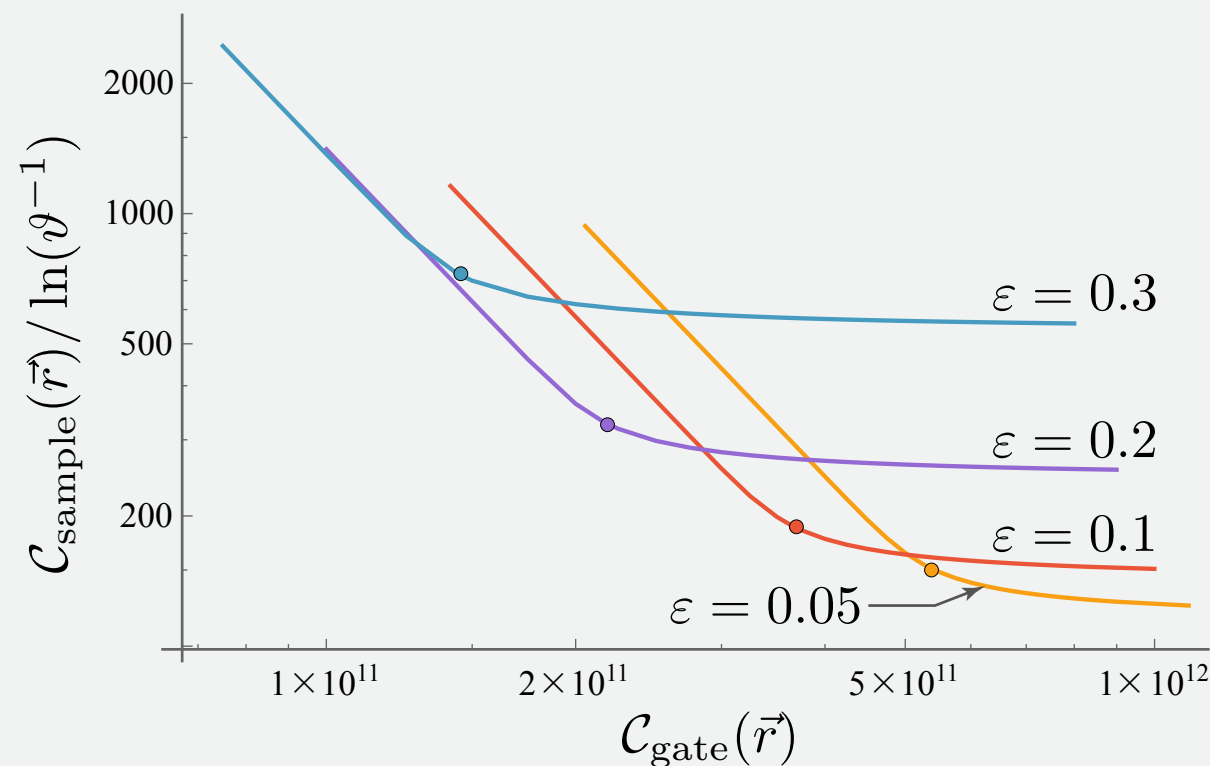


FeMoco benchmark

- Li et al. FeMoco Hamiltonian with 152 spin orbitals: 152+1=**153 qubits**
- Chemical accuracy $\Delta = 0.0016$ Hartree, one-norm $\lambda = 1511$ [Koridon et al., PRR (2021)]
- Gate complexity in single-qubit Pauli rotations $e^{i\theta P_l}$
- T gate or Toffoli-gate complexity similar
- Qubitization using heuristic truncations:

$$C_{gate} = 3.2 \cdot 10^{10} \text{ on 2196 qubits}$$

[Lee et al., PRX Quantum (2021)]



Hydrogen chains benchmark

- For length N chain, one-norm estimate $\lambda \approx O(N^{1.34})$ [Koridon et al., PRR (2021)]
- Our work $C_{gate} = \tilde{O}(N^{2.68}\Delta^{-2})$
- Qubitization based approaches:
 - A. rigorous $C_{gate} = \tilde{O}(N^{3.34}\Delta^{-1})$
 - B. sparse method $C_{gate} = \tilde{O}(N^{2.3}\Delta^{-1})$ [Berry et al., Quantum (2019)]
 - C. tensor hypercontraction method $C_{gate} = \tilde{O}(N^{2.1}\Delta^{-1})$ [Lee et al., PRX Quantum (2021)]
- Extensive properties $\Delta \propto N$ interesting for our methods: $C_{gate} = \tilde{O}(N^{0.68})$

Conclusion



Recap main result

- Given: n -qubit Hamiltonian $H = \sum_{l=1}^L \alpha_l P_l$ with $\lambda = \sum_{l=1}^L |\alpha_l|$, plus ansatz state ρ with ground state overlap $\langle \phi_0 | \rho | \phi_0 \rangle \geq \eta > 0$
- Output: ground state energy estimate \tilde{E}_0 with $|\tilde{E}_0 - E_0| \leq \Delta$
- **Result:** $n + 1$ qubits, $C_{gate} = \tilde{O}(\lambda^2 \Delta^{-2})$, $C_{sample} = \tilde{O}(\eta^{-2})$
- Advantages:
 - I. rigorous estimates
 - II. only depends on $\lambda \leq L$
 - III. only uses one ancilla
 - IV. flexible trade-off gate versus sample complexity
 - V. decrease error by solely taking more samples

Outlook: General matrix arithmetics

- General matrices A – instead of Hamiltonians H
- General functions $f(x)$ such as x^{-1} – instead of Heaviside function $\theta(x)$
- Goal to outperform state-of-the-art (probabilistic) classical methods with early fault-tolerance schemes
- Quantum singular value transformation (QSVT): $\|A\|_F$ or $s(A) \cdot \|A\|_{max}$
[Gilyen et al., STOC (2019)]
- Quantum random compiler (our approach):
 - no QRAM needed
 - $A = \sum_{l=1}^L \alpha_l P_l$ Paulis with $\lambda = \sum_{l=1}^L |\alpha_l|$ gives λ^2 complexity



Thank you!

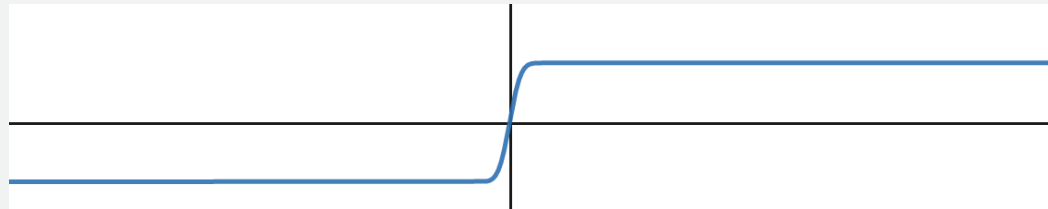
Extra slides



Extra: Proof Fourier series lemma

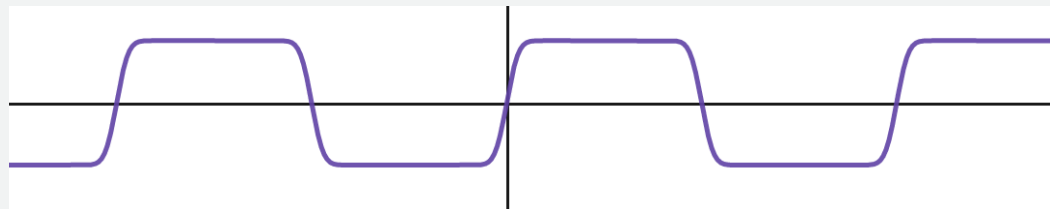
- Rigorous argument via truncated Chebyshev series of rescaled error function:

$$\operatorname{erf}(\beta y) = 2\pi^{-\frac{1}{2}} \int_0^{\beta y} e^{-t^2} dt \approx \sum_k c_k T_k(y) \quad [\text{Low \& Chuang, arxiv:1707.05391 (2017)}]$$



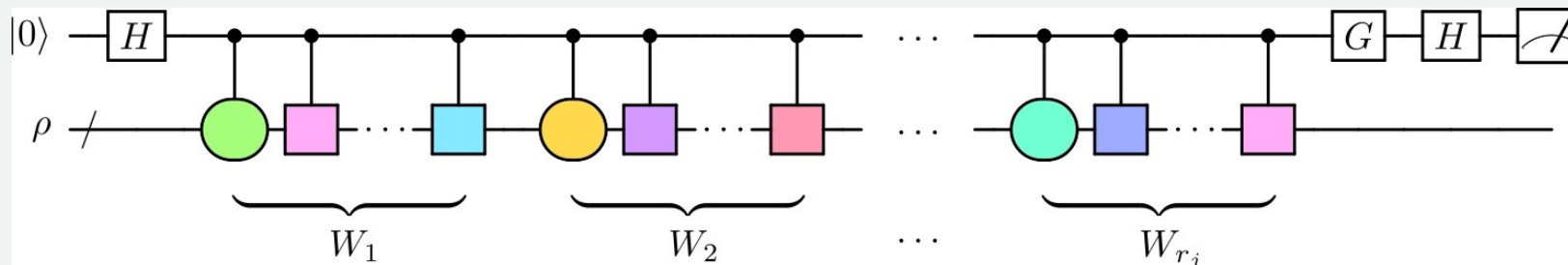
- Fourier series: $\Theta(x) \approx \operatorname{erf}(\beta \sin(x)) \approx \sum_k c_k T_k\left(\cos\left(\frac{\pi}{2} - x\right)\right)$

using $T_k(\cos(\cdot)) = \cos(k(\cdot))$



Extra: Proof random compiler lemma

- For $H = \sum_{l=1}^L \alpha_l P_l$ and $r \in \mathbb{N}$: $e^{iHt} = \left(e^{iHtr^{-1}} \right)^r = (1 + itr^{-1}H + \dots)^r$
 $1 + itr^{-1}H = \sum_{l=1}^L p_l (1 + itr^{-1}P_l) \propto \sum_{l=1}^L p_l e^{i\theta P_l}$ for $\theta = \arccos(\sqrt{1 + t^2 r^{-2}})$
- Similarly handle higher order terms – contain Paulis as well
- To sample U_k from $e^{iHt} = \sum_k b_k U_k$: independently sample r unitaries W_1, \dots, W_r from decomposition of $e^{iHtr^{-1}}$ and implement product



Extra: qDRIFT comparison

[Campbell, PRL (2019)]

- qDRIFT **approximates quantum channel**

$$\rho \mapsto e^{iHt} \rho e^{-iHt} \text{ for } H = \sum_{l=1}^L p_l P_l \text{ (normalized)}$$

by sampling r Paulis P_{l_1}, \dots, P_{l_r} independently with $\Pr[P_l] = p_l$ and putting

$$V := e^{itr^{-1}P_{l_1}} \dots e^{itr^{-1}P_{l_r}}$$

- qDRIFT compilation **error can only be suppressed by increasing gate count r**
- Our random compiler: approximates unitary $U = e^{iHt}$ and compilation error can be suppressed arbitrarily by simply taking more samples