

# Early Fault-Tolerant Quantum Algorithms for Matrix Functions via Trotter Extrapolation

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- **Practical Goal:** Achieve practical quantum advantage **despite hardware limitations** (limited qubits, circuit depth, and error).
- **Key Focus:** Develop algorithms with provable performance that are **resource-efficient** to be viable on existing quantum hardware.

- **The Computational Challenge:** Simulating quantum system is **intractable** for classical computers beyond few particles.

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  - $f(A) = \Theta_x(A) \rightarrow$  find the ground state energy using Phase Estimation.

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All these techniques use  $\text{Tr}[Ze^{iHT}]$  which we estimate with our algorithm.

# Background

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- **The Precision Challenge:**
  - Standard Trotterization requires a high number of steps ( $n$ ) for high precision ( $\varepsilon$ ), with error scaling poorly:
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  - This leads to deep circuits, limiting applicability on near-term hardware.

# Why Trotter for Early Fault Tolerance?

Method	Max Depth / Sample	Sample Overhead
Qubitization [4]	$\mathcal{O}\left(\Gamma\left[\Lambda T + \frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)}\right]\right)$	$\mathcal{O}(1/\varepsilon^2)$
Product Formulae [5]	$\mathcal{O}\left(\Gamma(\alpha_{\text{comm}}^{(p+1)})^{1/p} T^{1+1/p} \varepsilon^{-1/p}\right)$	$\mathcal{O}(1/\varepsilon^2)$
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- **Commutator scaling:** Errors scale with nested commutators, which are often small in realistic systems. Performs substantially better when  $\lambda_{\text{comm}} \ll \|H\|_1$

# Our Algorithm and Results

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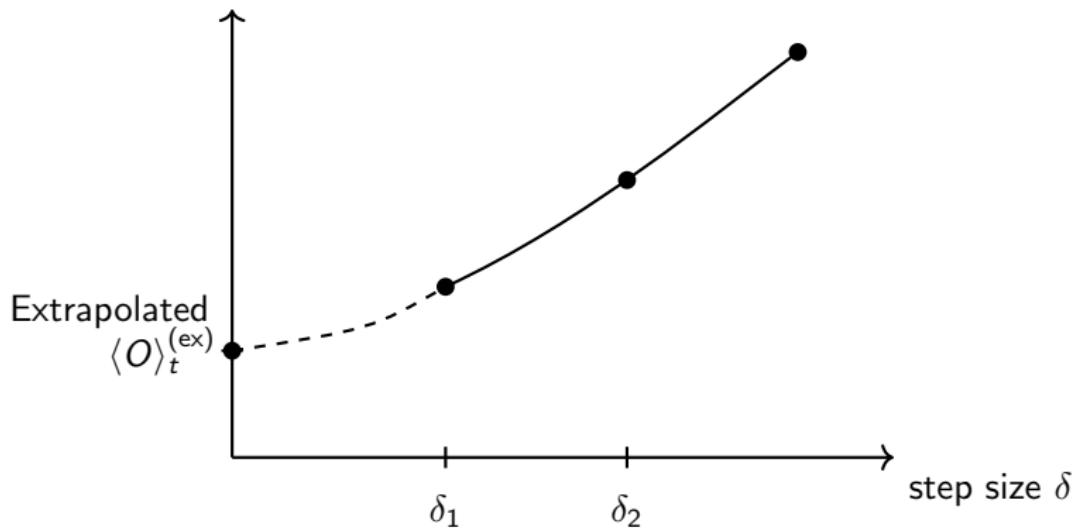
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- **Classical Extrapolation for Precision:**

- **Goal:** Improve error scaling without increasing quantum circuit depth.
- Perform quantum simulations at multiple Trotter step sizes and then **classically extrapolate** these results to for true evolution ( $\delta \rightarrow 0$ ).

Observable estimate  $\langle O \rangle_t$



# Comparisons with our Algorithm

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- **Key Question:** Can this be applied to matrix functions?

# Estimating General Matrix Functions

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We have it when  $Z = \rho$ , and extend to when  $\|Z\|_1$  is bounded.

## Richardson Extrapolation for each $\text{Tr}[Ze^{iAt_k}]$

For each  $t_k$ , estimate  $\text{Tr}[Ze^{iAt_k}]$  via Richardson-extrapolated circuits.

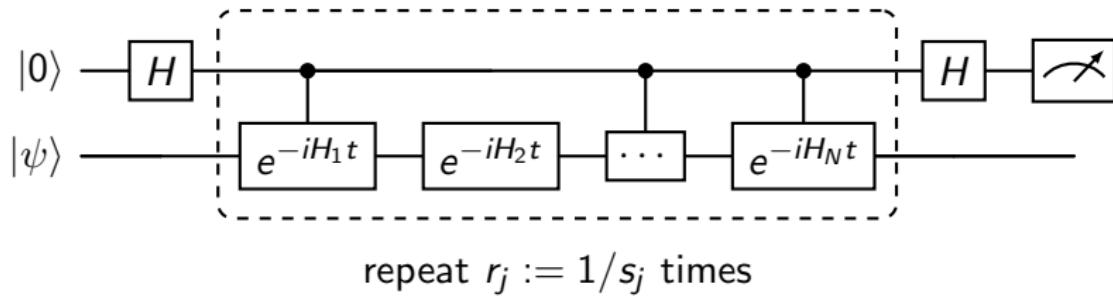
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Each  $\text{Tr}[Z\mathcal{P}^{1/s_j}(s_j t_k)]$  is estimated by sampling from Hadamard circuits like the one below:



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**Sample complexity**  $\mathcal{O}\left(\frac{\|Z\|_1^2 c^2 (\log \log(1/\varepsilon))^2}{\varepsilon^2} \cdot \log\left(\frac{1}{\delta}\right)\right)$

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- ② **Error Series Representation:**

$$\text{Tr} \left[ Z \mathcal{P}^{1/s}(sT) \right] = \text{Tr} \left[ Z e^{iAT} \right] + \sum_{j \in \sigma \mathbb{Z}_+ \geq p} s^j \text{Tr}[Z \tilde{E}_{j+1, K}(T)] + \text{Tr}[Z \tilde{F}_K(T, s)]$$

allows to use and analyze Richardson extrapolation (to get coefficients  $\{b_j\}_{j=1}^m$  and schedule  $\{s_j\}_{j=1}^m$ ) for improved gate complexity.

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- ① **Fourier Expansion:** to represent  $\text{Tr}[Zf(A)]$  term as a sum of  $\text{Tr}[Ze^{iHT}]$  terms.
- ② **Error Series Representation:**

$$\text{Tr} \left[ Z \mathcal{P}^{1/s}(sT) \right] = \text{Tr} \left[ Z e^{iAT} \right] + \sum_{j \in \sigma \mathbb{Z}_+ \geq p} s^j \text{Tr}[Z \tilde{E}_{j+1,K}(T)] + \text{Tr}[Z \tilde{F}_K(T, s)]$$

allows to use and analyze Richardson extrapolation (to get coefficients  $\{b_j\}_{j=1}^m$  and schedule  $\{s_j\}_{j=1}^m$ ) for improved gate complexity.

- ③ **Randomization:** improves sample overhead for circuits

# Applications

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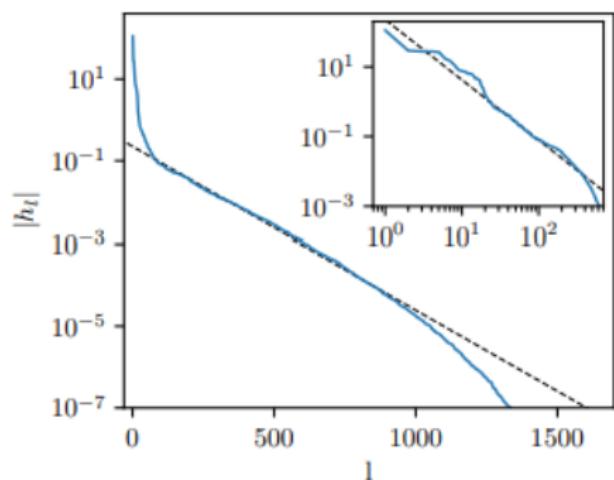
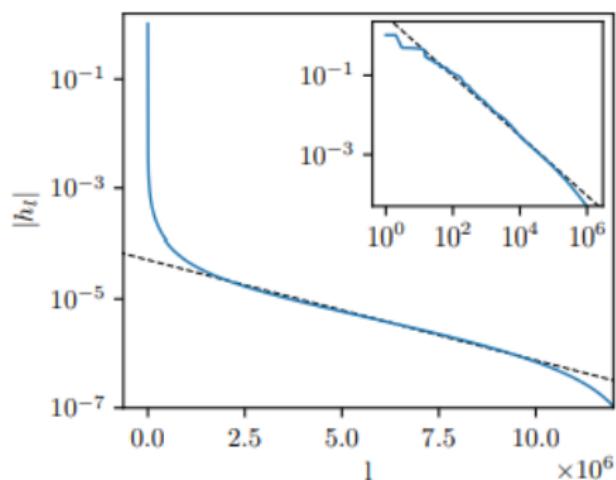
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# Refinements

# Partial Randomization Motivation

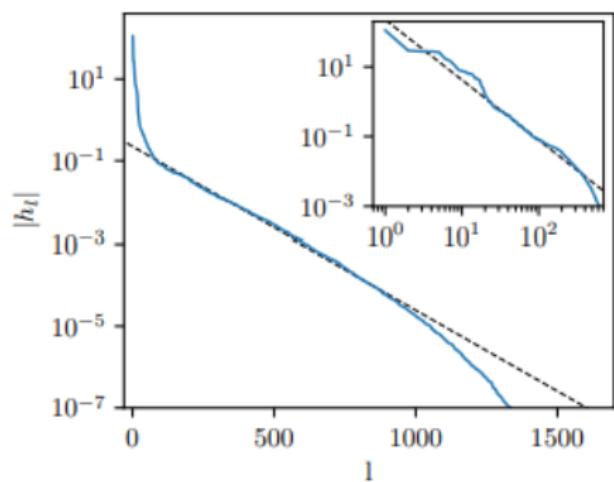
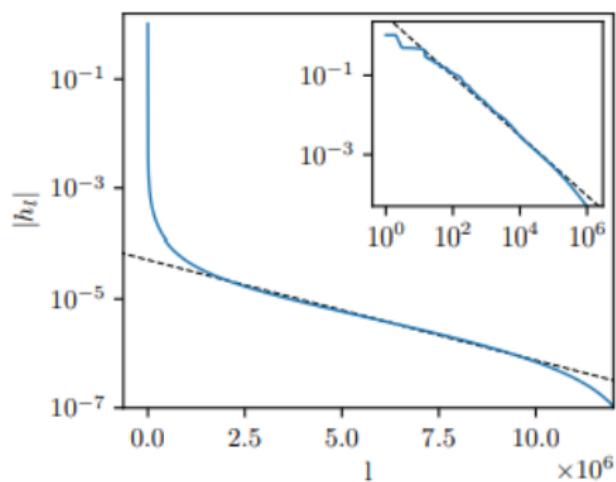
Many Hamiltonians have relatively few high-weight terms. <sup>1</sup>



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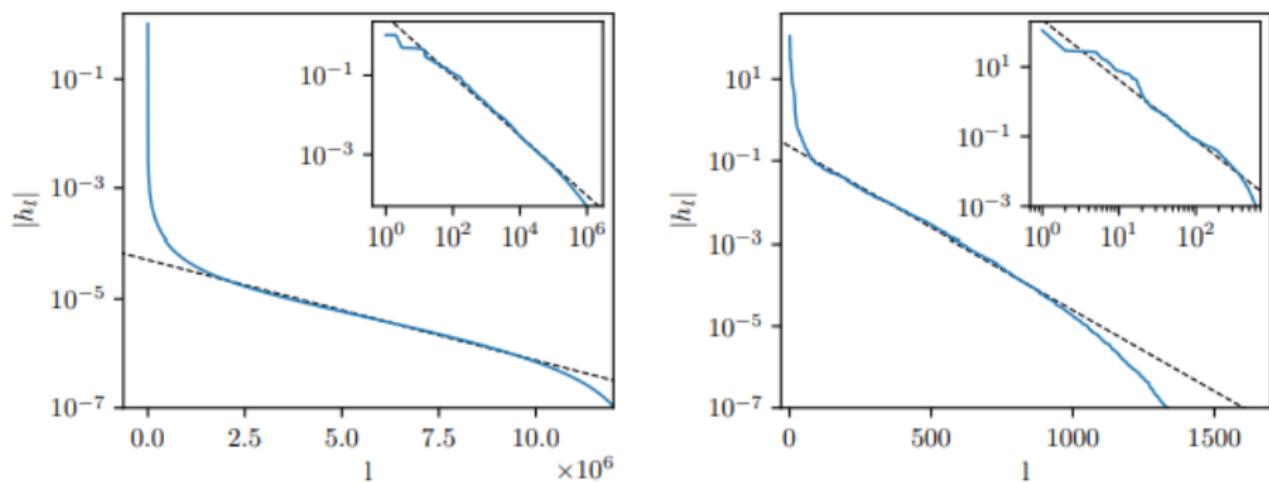


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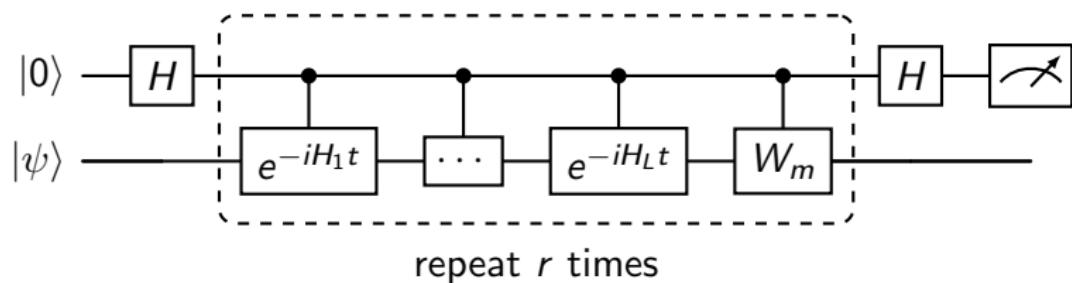


- The main plot shows exponential fit to the tail. ( $|h_\ell| \approx Ae^{-b\ell}$ )
- The insert shows power law fit for the large terms. ( $|h_\ell| \approx C \cdot \ell^{-\alpha}$ )

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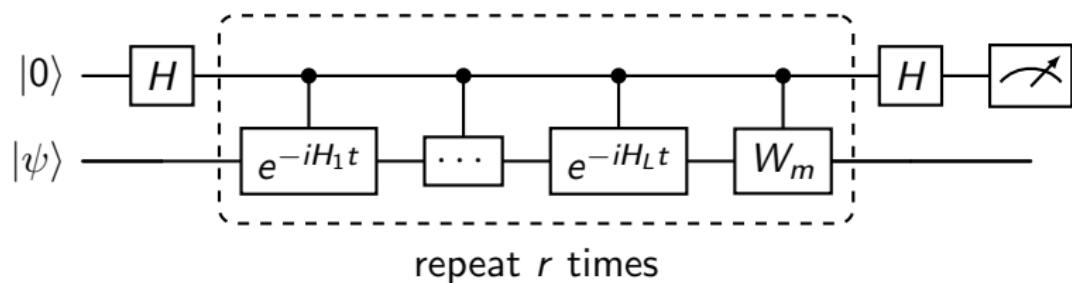
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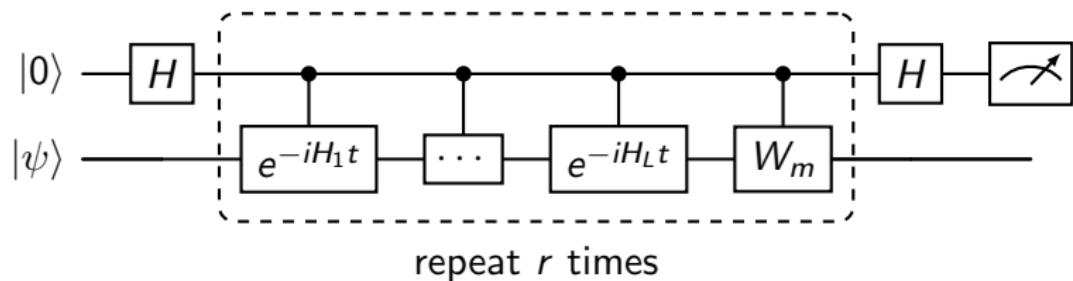
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To implement each  $W_m$  we use the Randomized Taylor Expansion [2].  
We apply Richardson-extrapolation on the partially random circuits for:

$$C_{\text{gate}} = \mathcal{O} \left( L_D (\Upsilon \lambda_{\text{comm}} T)^{1+\frac{1}{p}} \log^2 \left( \frac{1}{\varepsilon} \right) + \lambda_R^2 T^2 \right)$$

$$C_{\text{sample}} = \mathcal{O} \left( \frac{1}{\varepsilon^2} \left( \log \log \left( \frac{1}{\varepsilon} \right) \right)^2 \right)$$

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- Same bounds but with  $\lambda_{\text{comm}}^{(\eta)}$  defined from  $\alpha_{\text{comm}}^{(\eta)} < \alpha_{\text{comm}}$  [8]–[10] which are generally tighter than standard commutator bounds.

## Next Steps:

- **1D extrapolation:** Note that the sample complexity

$$C_{\text{sample}} = \mathcal{O} \left( \frac{1}{\varepsilon^2} \left( \log \log \left( \frac{1}{\varepsilon} \right) \right)^4 \right)$$

Can we improve the  $(\log \log(\frac{1}{\varepsilon}))^4$  to  $(\log \log(\frac{1}{\varepsilon}))^2$  by extrapolating directly over  $\text{Tr}[e^{iHT} \rho e^{-iHT'} O]$  instead of  $\text{Tr}[Ze^{iHT}]$ ?

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- **Analyzing constant factors** in the asymptotics for more specific performance estimates.

# Acknowledgments



**Samson Wang**

Thanks also to the rest of the Preskill Group, IQIM, and SFP for giving me such an enriching summer research experience.



**John Preskill**

Feedback:

**PLEASE LEAVE YOUR  
AUDIENCE FEEDBACK HERE**



# References I

- [1] L. Lin and Y. Tong, "Heisenberg-limited ground-state energy estimation for early fault-tolerant quantum computers," *PRX Quantum*, vol. 3, no. 1, Feb. 2022, ISSN: 2691-3399. DOI: 10.1103/prxquantum.3.010318. [Online]. Available: <http://dx.doi.org/10.1103/PRXQuantum.3.010318>.
- [2] K. Wan, M. Berta, and E. T. Campbell, "Randomized quantum algorithm for statistical phase estimation," , vol. 129, p. 030503, 3 Jul. 2022, 2110.12071. DOI: 10.1103/PhysRevLett.129.030503. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.129.030503>.
- [3] S. Wang, S. McArdle, and M. Berta, "Qubit-efficient randomized quantum algorithms for linear algebra," *PRX Quantum*, vol. 5, no. 2, Apr. 2024, ISSN: 2691-3399. DOI: 10.1103/prxquantum.5.020324. [Online]. Available: <http://dx.doi.org/10.1103/PRXQuantum.5.020324>.

## References II

- [4] G. H. Low and I. L. Chuang, "Hamiltonian simulation by qubitization," *Quantum*, vol. 3, p. 163, 2019, arXiv:1610.06546. DOI: 10.22331/q-2019-07-12-163.
- [5] A. M. Childs, Y. Su, M. C. Tran, N. Wiebe, and S. Zhu, "Theory of trotter error with commutator scaling," *Physical Review X*, vol. 11, no. 1, p. 011020, Feb. 2021. DOI: 10.1103/PhysRevX.11.011020. [Online]. Available: <http://dx.doi.org/10.1103/PhysRevX.11.011020>.
- [6] J. D. Watson and J. Watkins, *Exponentially reduced circuit depths using trotter error mitigation*, 2024. DOI: 10.48550/ARXIV.2408.14385. arXiv: 2408.14385. [Online]. Available: <https://arxiv.org/abs/2408.14385>.
- [7] J. Günther, F. Witteveen, A. Schmidhuber, M. Miller, M. Christandl, and A. Harrow, "Phase estimation with partially randomized time evolution," 2503.05647, 2025.

## References III

- [8] S. McArdle, E. Campbell, and Y. Su, "Exploiting fermion number in factorized decompositions of the electronic structure hamiltonian," *Physical Review A*, vol. 105, no. 1, Jan. 2022, ISSN: 2469-9934. DOI: 10.1103/physreva.105.012403. [Online]. Available: <http://dx.doi.org/10.1103/PhysRevA.105.012403>.
- [9] Y. Su, H. Y. Huang, and E. T. Campbell, "Nearly tight Trotterization of interacting electrons," , vol. 5, no. 1, pp. 1–58, 2021, 2012.09194, ISSN: 2521327X. DOI: 10.22331/Q-2021-07-05-495. arXiv: 2012.09194.
- [10] G. H. Low, Y. Su, Y. Tong, and M. C. Tran, "Complexity of implementing trotter steps," *PRX Quantum*, vol. 4, no. 2, May 2023, ISSN: 2691-3399. DOI: 10.1103/prxquantum.4.020323. [Online]. Available: <http://dx.doi.org/10.1103/PRXQuantum.4.020323>.