

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

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- **Key Focus:** Develop algorithms with provable performance that are **resource-efficient** to be viable on existing quantum hardware.

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 - $f(A) = A^{-1} \rightarrow$ solve linear systems and estimate Green's function
 - $f(A) = \Theta_x(A) \rightarrow$ 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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 - Standard Trotterization requires a high number of steps (n) for high precision (ε), 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

Applying Richardson Extrapolation on Trotter Formulas

- **Classical Extrapolation for Precision:**

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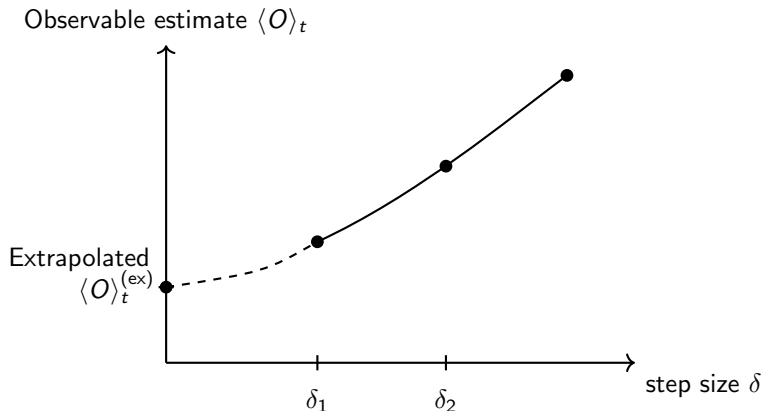
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- Perform quantum simulations at multiple Trotter step sizes and then **classically extrapolate** these results to for true evolution ($\delta \rightarrow 0$).



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

Estimating General Matrix Functions

Goal: Estimate physical observables of the form:

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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.

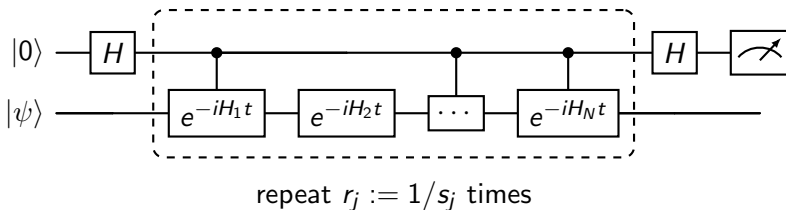
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Each $\text{Tr}[Z\mathcal{P}^{1/s_j}(s_j t_k)]$ is estimated by sampling from Hadamard circuits like the one below:



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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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Key Algorithmic Techniques

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

Applications

Ground Energy Estimation via QPE ($f(A) = \Theta_x(A)$)

Goal: Estimate the ground energy E_0 of a Hamiltonian H .

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① **Approximate CDF:** Construct the approximate CDF:

$$\tilde{C}(x) = \text{Tr}[\rho \tilde{\Theta}(xI - \kappa H)]$$

where $\tilde{\Theta}$ is a quantum filter approximating the Heaviside function.

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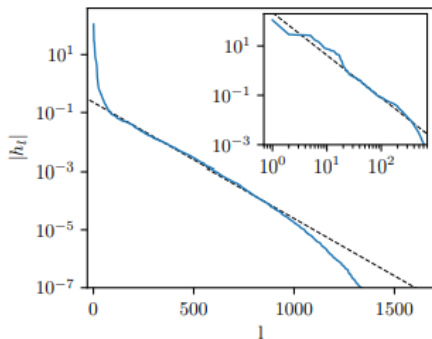
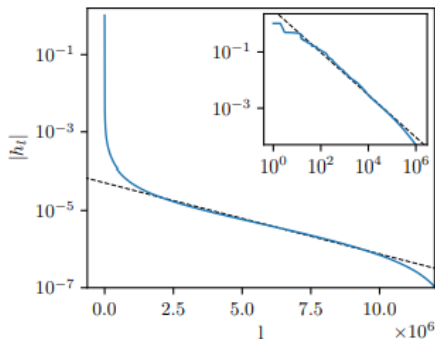
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Refinements

Partial Randomization Motivation

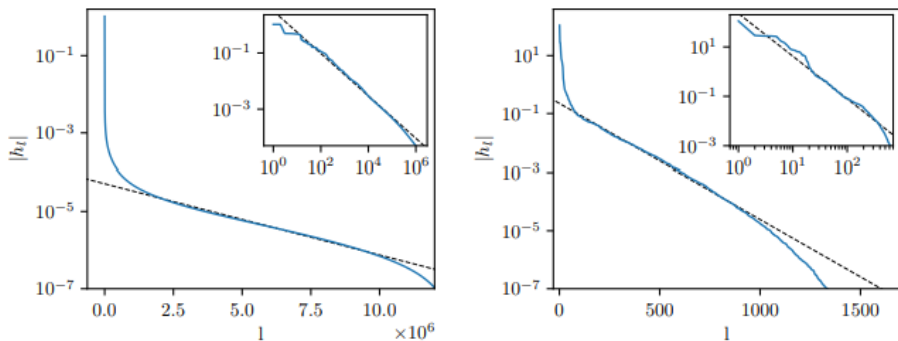
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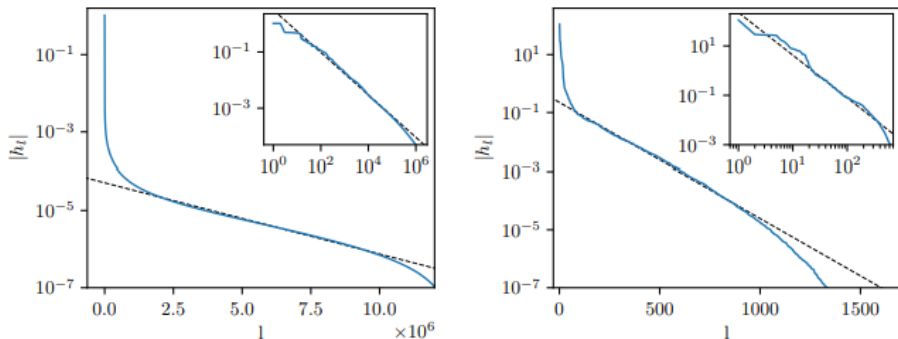


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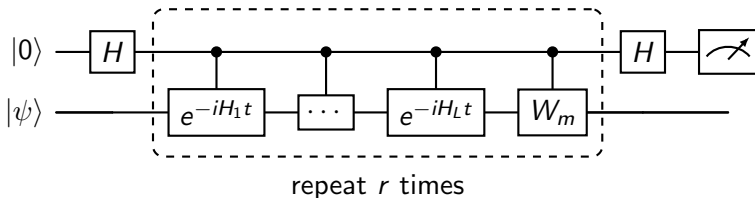


- The main plot shows exponential fit to the tail. ($|h_\ell| \approx Ae^{-b\ell}$)
- The insert shows power law fit for the large terms. ($|h_\ell| \approx C \cdot \ell^{-\alpha}$)

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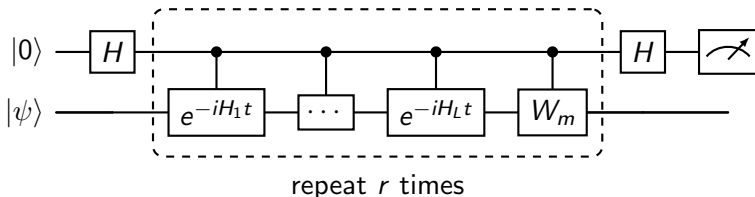
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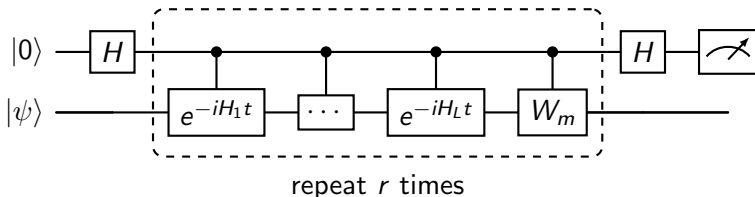
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We apply Richardson-extrapolation on the partially random circuits for:

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

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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

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

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

Acknowledgments



Samson Wang



John Preskill

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

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