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

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Background

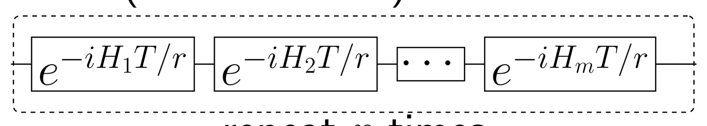
Product Formulae for Time Evolution

In a quantum system with Hamiltonian H, a state $|\psi(T)\rangle$ evolves as:

$$|\psi(T)\rangle = e^{-iHT/\hbar}|\psi(0)\rangle$$

When $H = \sum_{j=1}^{m} H_j$, we use product formulae (Trotterization) $\mathcal{P}$:

U(t) $\approx \left(\prod_{j=1}^{m} e^{-iH_jT/r}\right)^r$ or



- Each H_j is simple (e.g., a Pauli string), enabling native gate implementations.
- Number of steps: $r = \mathcal{O}\left((\alpha_{\text{comm}}^{(p+1)})^{\frac{1}{p}} T^{1+\frac{1}{p}} \varepsilon^{-\frac{1}{p}}\right)$.
- The order p controls the accuracy and scaling with time and error.

Why Product Formulae

Method	Max Depth / Sample	Sample Overhead
Product Formulae [1]	$\mathcal{O}\left(\Gamma(\alpha_{\text{comm}}^{(p+1)})^{1/p} T^{1+1/p} \varepsilon^{-1/p}\right)$	$\mathcal{O}(1/\varepsilon^2)$
Qubitization [2]	$\mathcal{O}\left(\Gamma\left[\Lambda T + \frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)}\right]\right)$	$\mathcal{O}(1/\varepsilon^2)$
Random Compiler [3]	$\mathcal{O}(\Lambda^2 T^2)$	$\mathcal{O}(1/\varepsilon^2)$

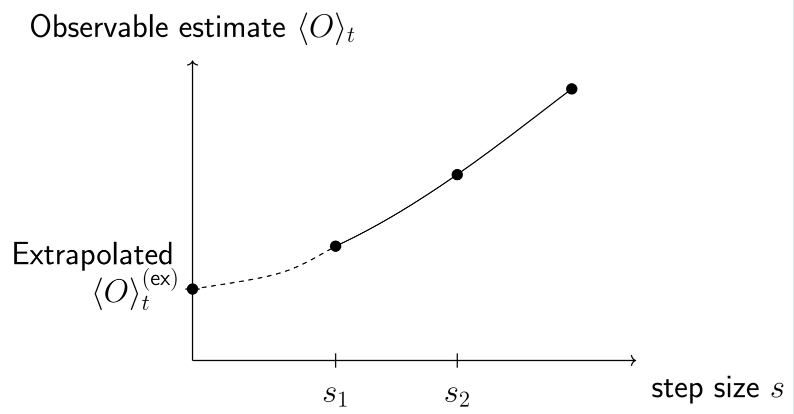
- **Low overhead:** No ancillas or block encoding required.
- **Simple compilation:** Native gate decomposition.
- **Commutator scaling:** Errors tied to size of nested commutators (generally small).
- **Limitation:** Trotter formulas scale poorly with ε.

Richardson Extrapolation

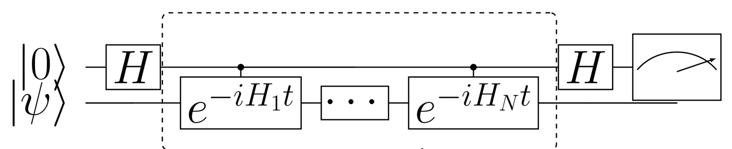
To reduce Trotter error, simulate with multiple step sizes $\delta_i = s_i T$ and extrapolate.

- **Improves accuracy:** Cancels error up to $\mathcal{O}(\delta^{m+1})$ with m runs.
- **Hardware-friendly:** Reduces circuit depth burden, by including more samples — ideal for EFT devices.
- Studied for time-evolved observables [4]. Does it work more generally?

Richardson Extrapolation for Trotter Observable



We create a linear combination of product formulae $\mathcal{P}$ using the Richardson schedule $\{s_j\}_{j=1}^{m}$ and coefficients $\{b_j\}_{j=1}^{m}$ to estimate Tr$[\rho e^{iHT}] \approx_{\varepsilon_R} \sum_{j=1}^{m} b_jTr[\rho\mathcal{P}(s_jT)]$. We estimate Tr$[\rho\mathcal{P}(s_jT)]$ using Hadamard tests (test for real part shown below):



Main Results

Key Takeaways

Richardson extrapolation provides an **exponential reduction** in the Trotter error scaling for **computing matrix functions**.

- Error scaling exponentially improves $\varepsilon^{-\frac{1}{p}} \to \log\left(\frac{1}{\varepsilon}\right)$ with only $\mathcal{O}\left(\log\log(\frac{1}{\varepsilon})^2\right)$ additional sample overhead
- $\lambda_{\text{comm}} = \sup_{\substack{j\in\sigma Z_+\geq\sigma m \\ 1\leq l\leq K}} \left(\sum_{\substack{j_1\ldots j_1\in\sigma Z_+\geq p \\ j_1+\cdots+j_l=j}} \prod_{\kappa=1}^{l} \frac{\alpha_{\text{comm}}^{(j_\kappa+1)}}{(j_\kappa+1)^2}\right)^{\frac{1}{(j+l)}}$
- Note that $\lambda_{\text{comm}} << \Lambda$ and bounded for useful Hamiltonians:
  1. electronic structure in plane-wave basis: $\alpha_{\text{comm}}^{(j)} = \mathcal{O}(n^j) \Rightarrow \lambda_{\text{comm}} = \mathcal{O}(n)$
  2. k-local: $\alpha_{\text{comm}}^{(j)} = \mathcal{O}\left(|||H|||_1^{j-1}\|H\|_1\right) \quad \Rightarrow \quad \lambda_{\text{comm}} = \mathcal{O}\left(|||H|||_1\|H\|_1^{\frac{1}{p+1}}\right)$

Compiling Primitives

We give an algorithm to estimate matrix functions using product formulas as primitives. Our simplest primitive to estimate Tr$[\rho e^{iHT}]$ has

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

Also have primitive for Tr$[e^{iHT}\rho e^{iHT'}O]$ with $\mathcal{O}\left(\frac{1}{\varepsilon^2}\log\log\left(\frac{1}{\varepsilon}\right)^4\right)$ sample complexity.

Using Fourier expansion $f(A) = \sum_{k=1}^{K} c_k e^{iAt_k}$, we use primitive to estimate Tr$[f(A)\rho]$

$$C_{\text{gate}} = \mathcal{O}\left(\Gamma\left(\Upsilon\lambda_{\text{comm}}T\right)^{1+\frac{1}{p}}\log\left(\frac{c(\varepsilon/3)}{\varepsilon}\right)\right), C_{\text{sample}} = \mathcal{O}\left(\frac{(c(\varepsilon/3))^2}{\varepsilon^2}\left(\log\log\left(\frac{1}{\varepsilon}\right)\right)^2\right)$$

and similarly Tr$[f(A)\rho f(A)^\dagger O]$ has $\mathcal{O}\left(\frac{(c(\varepsilon/3))^4}{\varepsilon^2}\left(\log\log\left(\frac{1}{\varepsilon}\right)\right)^4\right)$ sample complexity.

Algorithmic Applications

Phase Estimation

Estimates the ground energy E_0 of Hamiltonian H. We use our primitive as follows [5]:

- **Approximate CDF:** $\tilde{C}(x) = \mathrm{Tr}[\rho\,\tilde{\Theta}(xI - \kappa H)]$ with resolution parameter u and scaling κ where $\tilde{\Theta}$ is the approximated Heaviside function and κ is a normalization.
- **Ground State Energy Estimation:** By testing threshold crossings of $\tilde{C}(x \pm u)$, we can locate x^* such that $\left|\frac{x^*}{\kappa} - E_0\right| \leq \frac{u}{\kappa}$
- **Binary Search Strategy:** Iteratively narrow the search interval with $\mathcal{O}(\log(1/u))$ evaluations of $\tilde{C}(x)$, yielding an additive estimate of E_0.

Thus, to estimate E_0 to precision ε with constant success probability δ, we need:

$$C_{\text{gate}} = \tilde{\mathcal{O}}\left(\Gamma\left(\frac{\Upsilon\lambda_{\text{comm}}}{\varepsilon}\right)^{1+\frac{1}{p}}\right), \quad C_{\text{sample}} = \tilde{\mathcal{O}}\left(\frac{1}{\eta^2}\right)$$

where η is the initial state overlap.

Green's Function

In quantum physics, the frequency-domain Green's function describes how a system responds to perturbations at energy ω. It is essential for computing spectral properties, such as excitation energies and densities of states.

This function involves estimating the **resolvent operator** with our primitive:

$$R(\omega + i\Gamma_{\text{broad}}, \hat{H}) = (\omega + i\Gamma_{\text{broad}} - \hat{H})^{-1},$$

where $\Gamma_{\text{broad}} > 0$ is a broadening factor that ensures convergence.

$$C_{\text{gate}} = \tilde{\mathcal{O}}\left(\Gamma\left(a_{\max}\Upsilon\lambda_{\text{comm}}\frac{1}{\Gamma_{\text{broad}}}\right)^{1+\frac{1}{p}}\right), \quad C_{\text{sample}} = \tilde{\mathcal{O}}\left(\frac{1}{\Gamma_{\text{broad}}^2\varepsilon^2}\right).$$

Refinements and Extensions

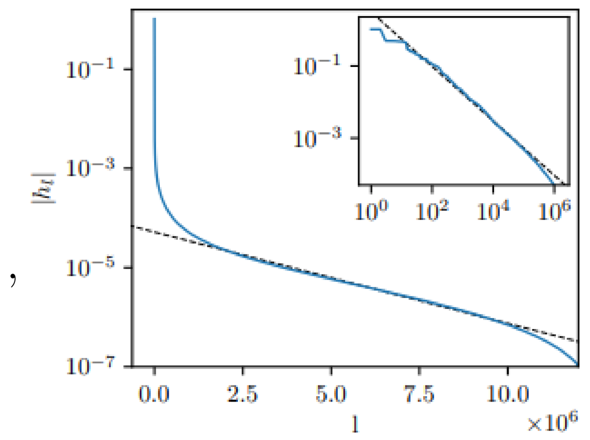
Partial Randomization [6]

Many Hamiltonians can be broken into a few high-weight terms, with the rest as low weights. We apply product formulas on L high weight terms and randomize the rest:

- Estimates Tr$[Ze^{iHT}]$
- We implement W_m using RTE.
- We apply Richardson-extrapolation for:

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

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



Fermion Systems

For systems in a η-fermion subspace, we tighten analysis with the fermionic semi-norm.

- Operators are number-preserving (map η-electron states to η-electron states)
- Gate complexity now dependent on the fermionic semi-norms of nested commutators
- Same bounds but with $\lambda_{\text{comm}}^{(\eta)}$ defined from $\alpha_{\text{comm}}^{(\eta)} < \alpha_{\text{comm}}$ [7, 8, 9]

References

[1] Childs et al., "Theory of Trotter Error with Commutator Scaling," 2021.
[2] Low et Chuang., "Hamiltonian Simulation by Qubitization," 2019.
[3] Wan et al., "Randomized Quantum Algorithm for Phase Estimation," 2021.
[4] Watson and Watkins.,"Exponentially Reduced Circuit Depths Using Trotter Error Mitigation," 2024.
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[7] Su et al., "Nearly tight Trotterization of interacting electrons," 2021.
[8] Mcardle et al., "Exploiting fermion number in factorized decompositions of the electronic structure Hamiltonian," 2022.
[9] Low et al. "On the complexity of implementing Trotter steps," 2023.