Title: Spectral analysis of product formulas for quantum simulation

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Abstract: Trotter-Suzuki formula is a practical and efficient algorithm for Hamiltonian simulation. It has been widely used in quantum chemistry, quantum field theory and condensed matter physics. Usually, its error is quantified by the operator norm distance between the ideal evolution operator and the digital evolution operator. However, recently more and more papers discovered that, even in large Trotter step region, the quantity of interest can still be accurately simulated. These robustness phenomena imply a different approach of analyzing Trotter-Suzuki formulas. In our previous paper, by analyzing the spectral analysis of the effective Hamiltonian, we successfully established refined estimations of digital errors, and thus improved the circuit complexity of quantum phase estimation and digital adiabatic simulation.

Spectral Analysis of Product Formulas for Quantum Simulation

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November 29, 2021

Outline

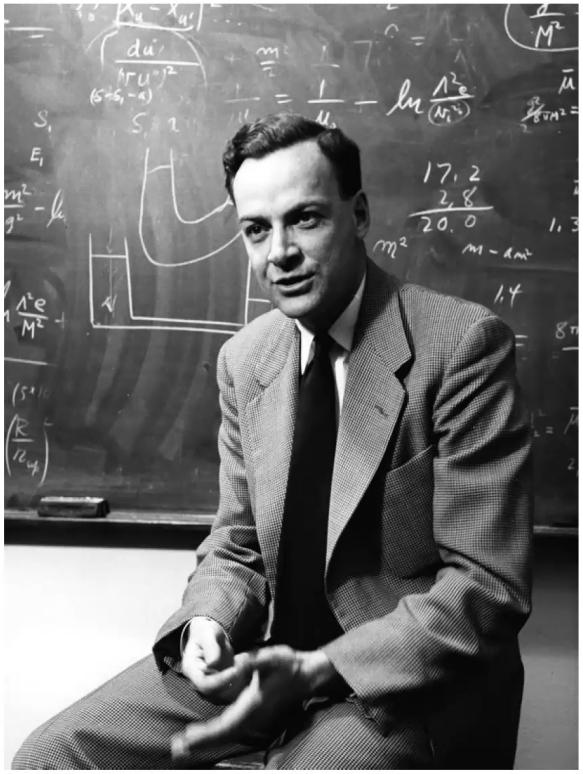
- Preliminaries about product formula
- Effective Hamiltonian method
- Application in quantum phase estimation
- Time-dependent Hamiltonian (digital adiabatic simulation)
- Discrete adiabatic process
- Robustness of local obseravable simulation

Quantum simulation

- The task of quantum simulation is to construct the time evolution operator in terms of local unitary gates

$$\frac{dU(t)}{dt} = -iHU(t) \rightarrow U(t) = e^{-iHt}$$

- Lots of applications : quantum chemistry, condensed-matter physics, high energy physics
- Different algorithms : product formulas, linear combination of unitaries, quantum signal processing



Preliminaries

- In product formula method, we replace each short time evolution operator $U(\delta t)$ with an approximation $U_{\text{tro}}(\delta t)$

$$U(t) = U(\delta t)^L \approx U_{\text{tro}}(\delta t)^L, \quad t = L\delta t$$

  L is termed as Trotter number, δt is a Trotter step

- For a general normalized Hamiltonian $H = \sum_{j=1}^{N} h_j, \|h_j\| \leq 1$, we separate the local terms into several layers $\{H_\gamma\}$, then the 1st order product formula gives

$$U_{\text{tro}}(\delta t) = \prod_{\gamma=1}^{\Gamma} e^{-iH_\gamma \delta t}$$

- There is a recursive way to write high order product formulas. The higher the order, the more accurate $U_{\text{tro}}(\delta t)$ is

Preliminaries

- The digital error of product formula method is quantified by the operator norm distance between $U(t)$ and $U_{\text{tro}}(\delta t)^L$

$$\Delta = \|U_{\text{tro}}(\delta t)^L - U(t)\|, \quad \|M\| = \max_{|x\rangle \neq 0} \frac{\|M|x\rangle\|_2}{\||x\rangle\|_2}$$

- Properties of operator norm

$$\|A|\psi\rangle\|_2 \leq \|A\|, \quad \|UA\| = \|A\|, \quad \|A+B\| \leq \|A\| + \|B\|$$

- The worst case vector norm distance is upper bounded by the operator norm distance

$$\|U_{\text{tro}}(\delta t)^L|\psi\rangle - U(t)|\psi\rangle\|_2 \leq \|U_{\text{tro}}(\delta t)^L - U(t)\|$$

Preliminaries

- The overall norm distance is related to that of a single step

$$\|U_{\text{tro}}(\delta t)^L - U(t)\| \leq L\|U_{\text{tro}}(\delta t) - U(\delta t)\|$$

- For 1st order product formula, it has been proved that [Childs et al., 21]

$$\|U_{\text{tro}}(\delta t) - U(\delta t)\| \leq \frac{1}{2}\sum_{\gamma}\|\sum_{\eta>\gamma}[H_\gamma, H_\eta]\|\delta t^2$$

  For 2-local Hamiltonian, the prefactor is proportional to N

- Based on ϵ, t, H, we determine the circuit depth L

$$\epsilon = O(L\delta t^2), \quad L = O(t^2/\epsilon)$$

Preliminaries

Simulation time	t
Size of Trotter step	δt
Trotter number	L
Number of sites	N
Expected error	ϵ
$\|U_{\text{tro}}(\delta t)^L - U(t)\|$	Δ

Table: Notations

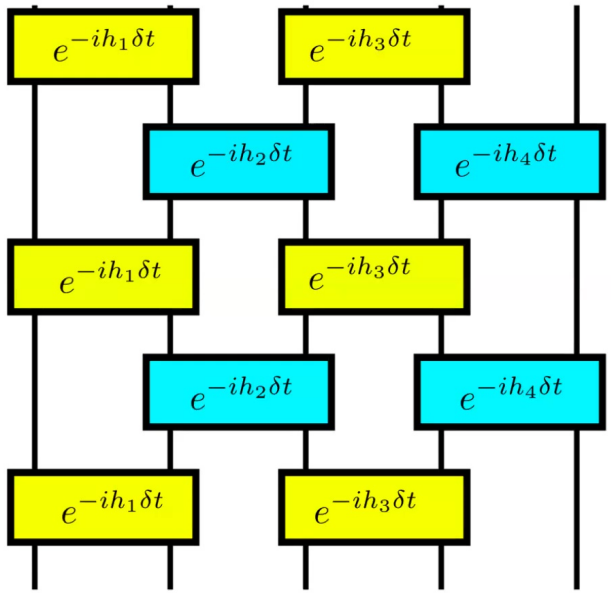


Figure: Quantum circuit of 1st order formula

Fidelity error

- Instead of analyzing the norm distance error Δ, we separate the error into fidelity error f and phase error θ

$$U_{\text{tro}}(\delta t)^L|\psi\rangle = \sqrt{1-f}e^{i\theta}U(t)|\psi\rangle + \sqrt{f}U(t)|\psi^{\perp}\rangle$$

- With $\Delta \leq 1/\sqrt{2}$,

$$f + \theta^2/4 \leq \Delta^2$$

- Theoretically, it's possible that $\sqrt{f}$ can be much smaller than Δ, as the digital error can be dominated by the phase error θ
- A trivial example is when the initial state is an eigenstate of H

Effective Hamiltonian method

- Each $U_{\text{tro}}(\delta t)$ can be regarded as an exact evolution under effective Hamiltonian

$$\widetilde{H} := i \log(U_{\text{tro}}(\delta t))/\delta t, \quad U_{\text{tro}}(\delta t)^L = e^{-i\widetilde{H}t}$$

  with spectral decomposition $\widetilde{H} = \sum_\ell \widetilde{E}_\ell \widetilde{P}_\ell$

- Use BCH formula, the leading term of $\widetilde{H}$ is

$$\widetilde{H} = H - \frac{i}{2}\sum_{\gamma<\eta}[H_\gamma, H_\eta]\delta t + O(\delta t^2)$$

- With eigenstate of H as initial state, the fidelity error is only relevant to the distance between eigenbasis

$$\sqrt{f_\ell} := \sqrt{1 - |\langle\psi_\ell|U^\dagger(t)U_{\text{tro}}(\delta t)^L|\psi_\ell\rangle|^2} \leq 2\|\widetilde{P}_\ell - P_\ell\|$$

  and it's irrelevant to the simulation time t

Effective Hamiltonian method

- Introduce

$$D := \sum_{\ell} e^{-i(\widetilde{E}_\ell - E_\ell)t} P_\ell, \quad \forall \ell, SP_\ell S^\dagger = \widetilde{P}_\ell$$

D encodes the deviation in energy levels, S encodes the deviation in eigenbasis

$$U_{\text{tro}}(\delta t)^L = SDU(t)S^\dagger$$

- Then Δ can be quantified in terms of $S - I$ and $D - I$

$$\begin{aligned}
\Delta &= \|SDU(t)S^\dagger - U(t)\| \\
&\leq \|SDU(t)S^\dagger - DU(t)\| + \|DU(t) - U(t)\| \\
&= \|[S, DU(t)]\| + \|D - I\| \\
&\leq 2\min\{\|S - I\|, \|DU(t) - I\|\} + \|D - I\|
\end{aligned}$$

Effective Hamiltonian method

- After simplification

$$\Delta \leq 2\sqrt{2}\max_{\ell}\|\widetilde{P}_\ell - P_\ell\| + \max_{\ell}|\widetilde{E}_\ell - E_\ell|t$$

  The first term is independent of t, the second term increases linearly with it

- Using perturbation theory and the expression of $\widetilde{H}$, we obtain

$$\|\widetilde{P}_\ell - P_\ell\| \leq \|\widetilde{H} - H\|/\lambda_\ell, \quad |\widetilde{E}_\ell - E_\ell| \leq \|\widetilde{H} - H\|$$

- $\|\widetilde{H} - H\|t$ is also a common estimation of Trotter error

$$\|e^{-i\widetilde{H}t} - e^{-iHt}\| \leq \|\widetilde{H} - H\|t$$

- The improvement originates in $|\widetilde{E}_\ell - E_\ell|$. Because of the specialty of $\widetilde{H} - H$, the perturbation in energy can be much smaller than the previous estimation

Improvement in $|\widetilde{E} - E|$

- In perturbation theory, $\delta E_\ell^{(1)} = \langle\psi_\ell|V|\psi_\ell\rangle$; if the leading term vanishes, the perturbation in energy will have order at most $O(\|V\|^2)$
- If the leading perturbation term of $\widetilde{H}$ is off-diagonal in the eigenbasis of H

$$\forall \ell, \quad \langle\psi_\ell|\widetilde{H} - H|\psi_\ell\rangle = O(\delta t^2),$$

then the Trotter error in energy is reduced from $O(\delta t)$ to $O(\delta t^2)$

$$|\widetilde{E}_\ell - E_\ell| = O\left(\delta t^2 \max\left\{1, \frac{1}{\lambda_\ell}\right\}\right)$$

- We find several general classes of Hamiltonian that satisfies this condition

Improvement in $|\widetilde{E} - E|$

- Recall that the leading perturbation in $\widetilde{H} - H$ is

$$\widetilde{H} - H = -\frac{i\delta t}{2} \sum_{\gamma<\eta} [H_\gamma, H_\eta] + O(\delta t^2)$$

- Two-layer case, $H = H_A + H_B$,

$$\langle \psi_\ell | [H_A, H_B] | \psi_\ell \rangle = \langle \psi_\ell | [H, H_B] | \psi_\ell \rangle = 0$$

- Real Hamiltonian, real symmetric matrix has real vectors as eigenstates

$$\langle \psi_\ell | H_\eta H_\gamma | \psi_\ell \rangle = \langle \psi_\ell | H_\gamma H_\eta | \psi_\ell \rangle$$

Comparison between 1st and 2nd order product formulas

- The 1st and 2nd order product formulas can share similar asymptotic scalings under certain conditions [Tran et.al, 2020]
- 2nd order product formula has expression

$$U_{\text{tro}}^{(2)}(\delta t)^L := \left(\prod_{\gamma=1}^{\Gamma} e^{-iH_\gamma \delta t/2}\right)\left(\prod_{\gamma=\Gamma}^{1} e^{-iH_\gamma \delta t/2}\right)$$

  It has been proved that $\|U_{\text{tro}}^{(2)}(\delta t)^L - U(t)\| = O(L\delta t^3)$
- With the improvement in $|\widetilde{E}_\ell - E_\ell|$, we obtain a similar result [Yi, Crosson, 21]

$$\|U_{\text{tro}}(\delta t)^L - U(t)\| = O(a \cdot \delta t) + O(b \cdot L\delta t^3)$$

Application in quantum phase estimation

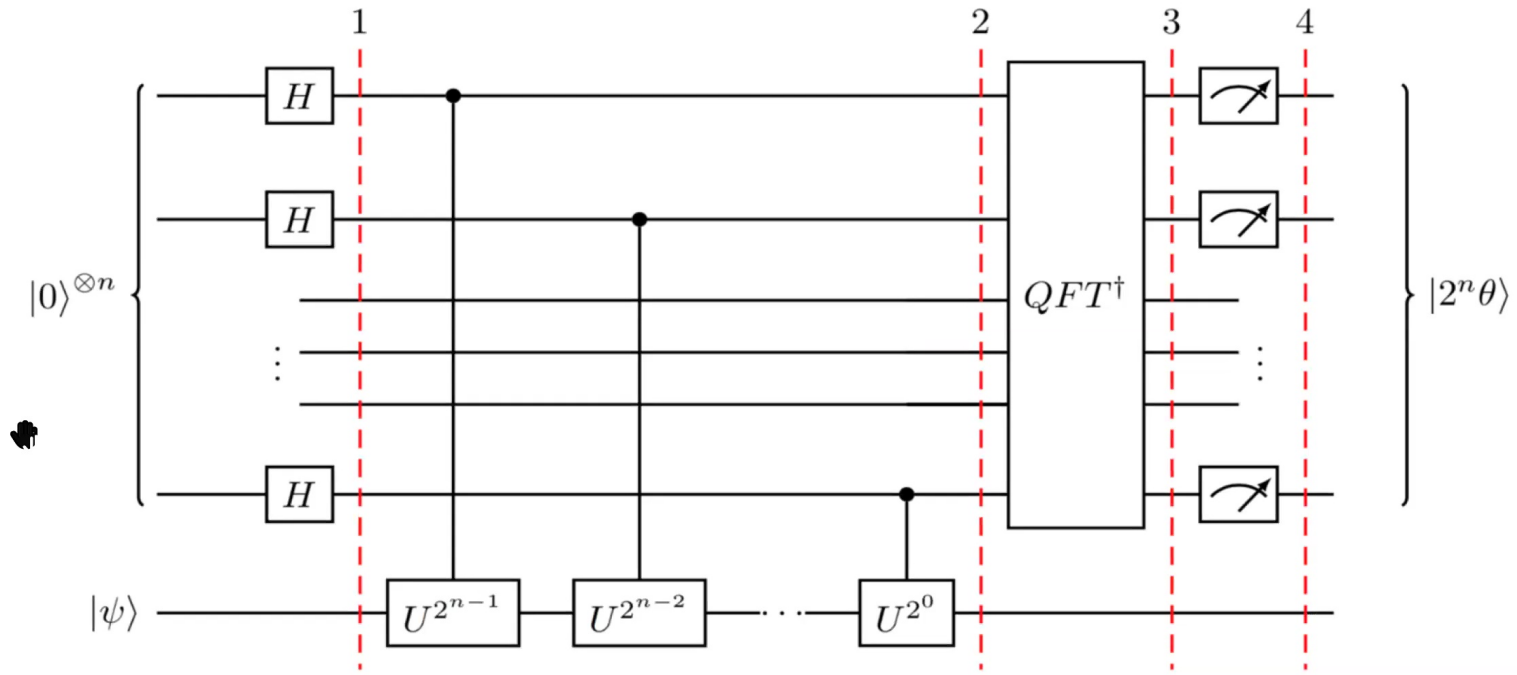


Figure: Circuit of Quantum Phase Estimation

Application in quantum phase estimation

- Write the effective initial state of the Trotterized unitary operator as $|\widetilde{\psi}\rangle$

$$|\psi\rangle = \sqrt{1-p}|\widetilde{\psi}\rangle^{\mathbb{I}} + \sqrt{p}|\widetilde{\psi}^{\perp}\rangle$$

- The success rate should be decreased by a factor of $(1-p)$, which is negligible
- To make sure the phase error is smaller than precision ξ, there should be a restriction on the size of Trotter step

$$|\widetilde{E} - E|t_0 \leq 2\pi\xi$$

- Our method also applies to other phase estimation algorithms as well [Russo et.al, 20], as long as Trotterized unitary operator is used

Application in quantum phase estimation

- [Yi, Crosson, 21] Suppose there's a quantum circuit that performs quantum phase estimation using 1st order Trotter formula, the size of the register is n thus the precision is $\xi = 2^{-n}$. The unitary operator is $U = e^{-iHt_0}$ where H is supported on N qubits and satisfies one of the conditions that reduces Trotter error in energy, to guarantee $|\widetilde{E} - E|t_0 \leq 2\pi\xi$, we require

$$\delta t = O\left(\frac{1}{N}\sqrt{\frac{\xi}{t_0}}\min\{1,\lambda\}\right), \quad L = O\left(N\sqrt{\frac{t_0^3}{\xi}}\max\left\{1,\frac{1}{\lambda}\right\}\right)$$

- Here L represents the circuit depth of a single U
- Without the improvement in $|\widetilde{E} - E|$,

$$L = O\left(\frac{Nt_0^2}{\xi}\right)$$

Summary

- $$U_{\text{tro}}(\delta t)^L = e^{-i\widetilde{H}t} = SDU(t)S^\dagger$$
$$\Delta \leq 2\|S - I\| + \|D - I\|$$

- Because of the specialty of the perturbation part $\widetilde{H} - H$, the deviation in energy levels can be a lot smaller than the estimation $|\widetilde{E}_\ell - E_\ell| \leq \|\widetilde{H} - H\|$
- Using this framework, we obtain improvements in the error estimation of 1st order product formula and the circuit depth of quantum phase estimation
- Q : However, the inverse dependence on λ doesn't show up in other analysis, which might be eliminated by further analysis

Time-dependent quantum simulation

- For time-dependent Hamiltonian [Poulin et.al, 11],

$$
\begin{aligned}
U(t) &= \prod_{j=1}^{L} \exp_{\mathcal{T}} \left(-i \int_{t_j}^{t_j+\delta t} \sum_{\gamma=1}^{\Gamma} H_\gamma(\tau) d\tau \right) \\
&\approx \prod_{j=1}^{L} \prod_{\gamma=1}^{\Gamma} \exp_{\mathcal{T}} \left(-i \int_{t_j}^{t_j+\delta t} H_\gamma(\tau) d\tau \right) \quad \text{Trotter splitting, } \epsilon' = O(L\delta t^2) \\
&\approx \prod_{j=1}^{L} \prod_{\gamma=1}^{\Gamma} \exp\left(-iH_\gamma(t_j + \delta t/2) \cdot \delta t\right) \quad \text{Averaged approximation, } \epsilon'' = O(L\delta t^2)
\end{aligned}
$$

Digital adiabatic simulation

- The simulation of adiabatic process is an important step in adiabatic quantum computing
- Solution to computational problems can be encoded in the ground state of a Hamiltonian

$$H = -\sum_{jk} J_{jk} Z_j Z_k - \sum_k h_k Z_k$$

  e.g. MAX-CUT, spin glass
- Ground state of a complicated Hamiltonian can be generated by adiabatic evolution
- Adiabatic theorem (informal): set the ground state of initial Hamiltonian as the initial state, if the Hamiltonian evolves with time slowly enough, the evolved state will approximately be the ground state of the Hamiltonian at the corresponding time

Digital adiabatic simulation

- Linear adiabatic path : $\hat{H}(t) = (1 - \frac{t}{T})H_i + \frac{t}{T}H_f, t \in [0, T]$, e.g.

$$H_i = -\sum_j X_j, \quad |0_i\rangle = |+\rangle^{\otimes N}$$

- T quantifies how slow the evolution is, the adiabatic limit is

$$A(T) = \exp_{\mathcal{T}}\left(-i\int_0^T \hat{H}(\tau)d\tau\right)$$

$$\lim_{T\to\infty} A(T)|0_i\rangle = |0_f\rangle$$

Digital adiabatic simulation

- Simplify the previous expression with a dimensionless variable $s = t/T$

$$H(s) = \hat{H}(Ts) = (1-s)H_i + sH_f$$

$$A(T) = \exp_{\mathcal{T}}\left(-iT\int_0^1 H(s)ds\right)$$

- Adiabatic theorem (formal) [Jensen et al., 07]: the inaccuracy of adiabatic evolution is quantified by the fidelity distance

$$\epsilon_{\text{adb}} = \sqrt{1 - |\langle 0_f|A(T)|0_i\rangle|^2}$$

$$\epsilon_{\text{adb}} \leq \mathcal{G}(T,H) = O\left(\frac{\max\|H'(s)\|}{T\min\lambda(s)^2}\right)$$

Perform DAS using product formula

- Step 1, discretization

$$A_d = \prod_{j=0}^{L} U_j, \quad U_j = e^{-iH_j \delta t}, \quad s_j = j/L$$

$$\delta t = \frac{T}{L}, \quad H_j = (1 - s_j) H_i + s_j H_f$$

- Step 2, Trotter splitting

$$A_{\text{tro}} = \prod_{j=0}^{L} \widetilde{U}_j$$

$$\widetilde{U}_j = e^{-i(1-s_j)H_i \delta t} e^{-i s_j H_f \delta t}$$

Evolution time	T
Trotter number	L
Size of Trotter step	δt
Ideal adiabatic operator	$A(T)$
Discrete adiabatic operator	A_d
Trotterized adiabatic operator	A_{tro}

Errors in DAS

- The error estimated by adiabatic theorem is

$$\epsilon_{\text{adb}} = \sqrt{1 - |\langle 0_f|A(T)|0_i\rangle|^2} = \mathcal{G}(T, H) = O\left(\frac{\|H'\|}{T\lambda^2}\right)$$

- The error originated from prodcut formula is

$$\epsilon_{\text{tro}} = \sqrt{1 - |\langle 0_i|A^\dagger(T)A_{\text{tro}}|0_i\rangle|^2} \leq \|A(T) - A_{\text{tro}}\| = O\left(\max_{\tau,\gamma}\|H_\gamma(\tau)\|\frac{T^2}{L}\right)$$

- If we only focus on the parameter scaling of L, T, then

$$\epsilon_{\text{tot}} = \sqrt{1 - |\langle 0_f|A_{\text{tro}}|0_i\rangle|^2} \leq \epsilon_{\text{adb}} + \epsilon_{\text{tro}} = O\left(\frac{1}{T}\right) + O\left(\frac{T^2}{L}\right)$$

Robustness of DAS

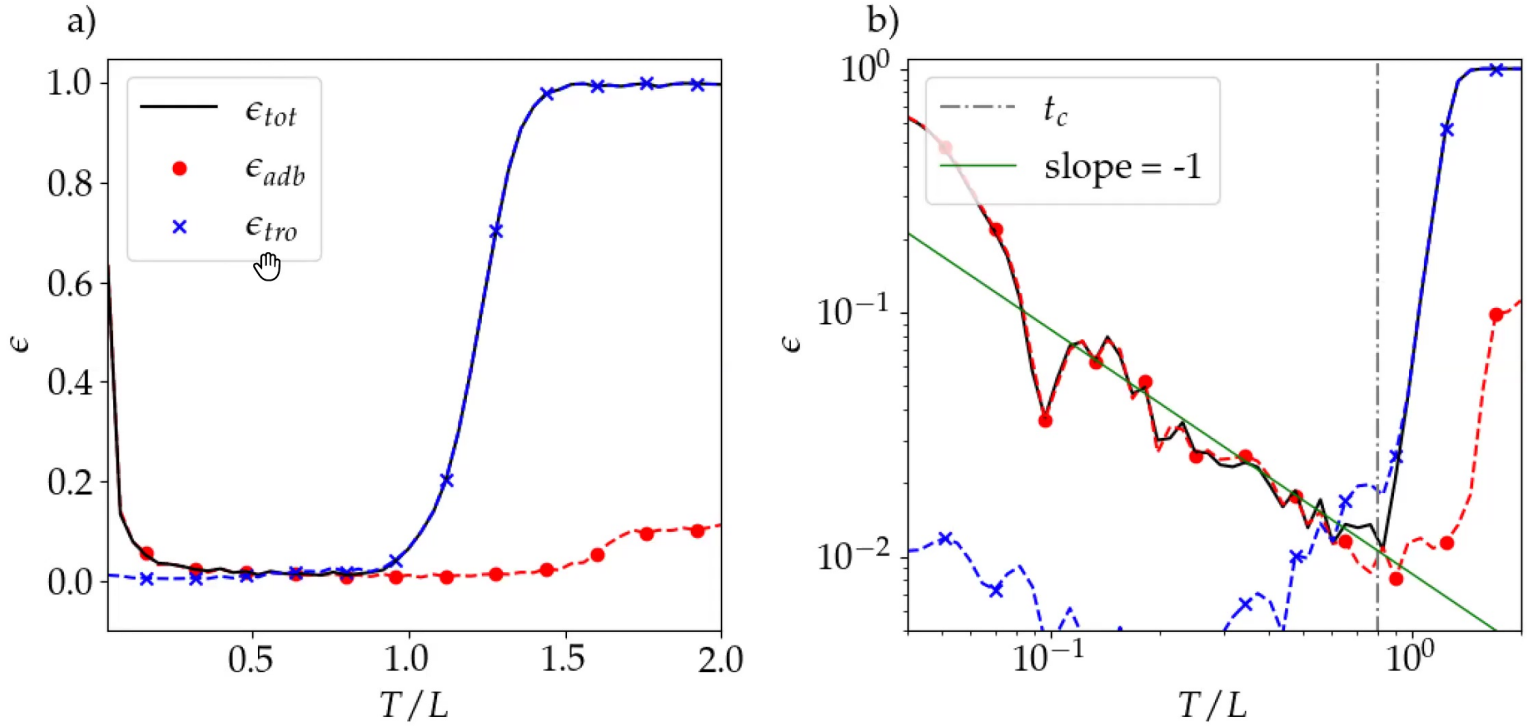


Figure: Total error of DAS. $H_i = -\sum_{j=1}^{N} X_j$, $H_f = -\sum_{j=1}^{N}(0.5 Z_j Z_{j+1} + Z_j)$ with OBC. $N = 8$. $L = 100$

Errors in DAS

- The error estimated by adiabatic theorem is

$$\epsilon_{\text{adb}} = \sqrt{1 - |\langle 0_f|A(T)|0_i\rangle|^2} = \mathcal{G}(T, H) = O\left(\frac{\|H'\|}{T\lambda^2}\right)$$

- The error originated from prodcut formula is

$$\epsilon_{\text{tro}} = \sqrt{1 - |\langle 0_i|A^\dagger(T)A_{\text{tro}}|0_i\rangle|^2} \leq \|A(T) - A_{\text{tro}}\| = O\left(\max_{\tau,\gamma}\|H_\gamma(\tau)\|\frac{T^2}{L}\right)$$

- If we only focus on the parameter scaling of L, T, then

$$\epsilon_{\text{tot}} = \sqrt{1 - |\langle 0_f|A_{\text{tro}}|0_i\rangle|^2} \leq \epsilon_{\text{adb}} + \epsilon_{\text{tro}} = O\left(\frac{1}{T}\right) + O\left(\frac{T^2}{L}\right)$$

Robustness of DAS

- The ϵ_{tro} calculated here is the fidelity error instead of operator norm error. We didn't see the scaling $\epsilon_{\text{tro}} = O(T^2/L)$. The previous estimation is not accurate
- The inverse dependence of T remains true for large Trotter steps, which we call it as the robustness of DAS
- The meaning is, in large Trotter step region, A_{tro} already deviates a lot from $A(T)$, while the quantity of interest is still accurate; this is because for some specific quantum simulation task, we only need part of the information in the unitary operators
- We can use the effective Hamiltonian argument to obtain a new upper bound

Effective adiabatic path

- The Trotterized evolution operator A_{tro} is an exact adiabatic evolution under

$$\widetilde{H}(s,\delta t) = i\log(\widetilde{U}(s))/\delta t$$

$$\widetilde{A}(T) = \exp_{\mathcal{T}}\left(-iT\int_0^1 \widetilde{H}(s,\delta t)ds\right) \approx A_{\text{tro}}$$

- If $\widetilde{H}(s,\delta t)$ satisfies the boundary condition

$$\widetilde{H}(0,\delta t) = H_i, \quad \widetilde{H}(1,\delta t) = H_f$$

It's natural to apply adiabatic theorem on the new path as another upper bound

$$\epsilon_{\text{tot}} = O\left(\sqrt{1-|\langle 0_f|\widetilde{A}(T)|0_i\rangle|^2}\right) = O(\mathcal{G}(T,\widetilde{H}))$$

Discrete adiabatic process

- Consider a discrete adiabatic evolution operator of a general adiabatic path $H(s)$

$$A_d = \prod_{j=0}^{L} U_j, \quad U_j = e^{-iH(s_j)T/L}$$

- The evolved state can be written as

$$A_d|0_i\rangle = e^{-i\theta_A}\left(\sqrt{1-\epsilon_{\text{adb}}^2}|0_f\rangle + \sum_{\ell\neq 0}\epsilon_\ell|\ell_f\rangle\right)$$

- Later we will see that θ_A and ϵ_ℓ have very different properties

Discrete adiabatic process

- Outline of proof [Yi, 21]

$$
\begin{aligned}
\langle 0_f|A_d|0_i\rangle &= \langle 0_f|\prod_j e^{-iH(s_j)T/L}|0_i\rangle \\
&= e^{-i\theta_A}\langle 0_f|\prod_j e^{-i(H(s_j)-E_0(s_j))T/L}|0_i\rangle, \quad \theta_A = \frac{T}{L}\sum_j E_0(s_j) \\
&= e^{-i\theta_A}\langle 0_f|\prod_j D_j\Lambda_j D_j^\dagger|0_i\rangle \\
&= e^{-i\theta_A}\langle 0_f|D_L\Gamma D_0^\dagger|0_i\rangle, \quad \Gamma = \Lambda_L\prod_j(D_{j+1}^\dagger D_j\Lambda_j) \\
&= e^{-i\theta_A}\Gamma_{00}
\end{aligned}
$$

Discrete adiabatic process

- In the matrix form

$$\Gamma = \begin{pmatrix} \sqrt{1-\epsilon_{\text{adb}}^2} & \cdot & \cdot & \cdot \\ \epsilon_1 & \cdot & \cdot & \cdot \\ \epsilon_2 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}, \quad \epsilon_{\text{adb}}^2 = \sum_{\ell>0} |\epsilon_\ell|^2$$

- Perform linear expansion of Γ

$$\Gamma = \prod_{j=0}^{L} \Lambda_j + \sum_{j=0}^{L} \left(\prod_{k>j} \Lambda_j \right) (D_{j+1}^\dagger D_j - I) \left(\prod_{k<j} \Lambda_j \right) + \cdots$$

- It's required that the phases of the eigenbasis of $H(s)$ are chosen to let the transition matrix between them $D_{j+1}^\dagger D_j$ closest to identity

Discrete adiabatic process

- Outline of proof [Yi, 21]

$$
\begin{aligned}
\langle 0_f|A_d|0_i\rangle &= \langle 0_f|\prod_j e^{-iH(s_j)T/L}|0_i\rangle \\
&= e^{-i\theta_A}\langle 0_f|\prod_j e^{-i(H(s_j)-E_0(s_j))T/L}|0_i\rangle, \quad \theta_A = \frac{T}{L}\sum_j E_0(s_j) \\
&= e^{-i\theta_A}\langle 0_f|\prod_j D_j\Lambda_j D_j^\dagger|0_i\rangle \\
&= e^{-i\theta_A}\langle 0_f|D_L\Gamma D_0^\dagger|0_i\rangle, \quad \Gamma = \Lambda_L\prod_j(D_{j+1}^\dagger D_j\Lambda_j) \\
&= e^{-i\theta_A}\Gamma_{00}
\end{aligned}
$$

Discrete adiabatic process

- In the matrix form

$$\Gamma = \begin{pmatrix} \sqrt{1-\epsilon_{\text{adb}}^2} & \cdot & \cdot & \cdot \\ \epsilon_1 & \cdot & \cdot & \cdot \\ \epsilon_2 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}, \quad \epsilon_{\text{adb}}^2 = \sum_{\ell>0} |\epsilon_\ell|^2$$

- Perform linear expansion of Γ

$$\Gamma = \prod_{j=0}^{L} \Lambda_j + \sum_{j=0}^{L} \left(\prod_{k>j} \Lambda_j \right) (D_{j+1}^\dagger D_j - I) \left(\prod_{k<j} \Lambda_j \right) + \cdots$$

- It's required that the phases of the eigenbasis of $H(s)$ are chosen to let the transition matrix between them $D_{j+1}^\dagger D_j$ closest to identity

Discrete adiabatic process

- Using the linear expansion, we obtain the undesired transition amplitudes

$$\epsilon_\ell \approx \frac{1}{L}\sum_{j=0}^{L-1}\frac{\langle \ell(s_j)|H'(s_j)|0(s_j)\rangle}{\lambda_\ell(s_j)}\exp\left[-i\frac{T}{L}\sum_{k<j}\lambda_\ell(s_k)\right], \quad \lambda_\ell = E_\ell - E_0$$

- Consider its continuous limit

$$\lim_{L\to\infty}\epsilon_\ell = \int_0^1 \frac{\langle \ell(s)|H'(s)|0(s)\rangle}{\lambda_\ell(s)}\exp[-iT\int_0^s \lambda_\ell(s')ds']ds$$

- Use Riemann-Lebesgue lemma (integration by part)

$$|\epsilon_\ell| = O\left(\frac{\|H'(s)\|}{T\lambda_\ell^2(s)}\right)$$

Robustness of discrete Riemann-Lebesgue lemma

- Riemann-Lebesgue lemma

$$I = \int_0^1 f(s)\exp[-iTg(s)]ds, \quad g'(s) > 0, \quad |I| = O\left(\frac{|f(s)|}{T|g'(s)|}\right)$$

- Consider a specific example with $f(s) = 1, g(s) = s$

$$I = \int_0^1 e^{-iTs}ds = \frac{1-e^{-iT}}{iT}, \quad |I| = \frac{|\sin(T/2)|}{T/2}$$

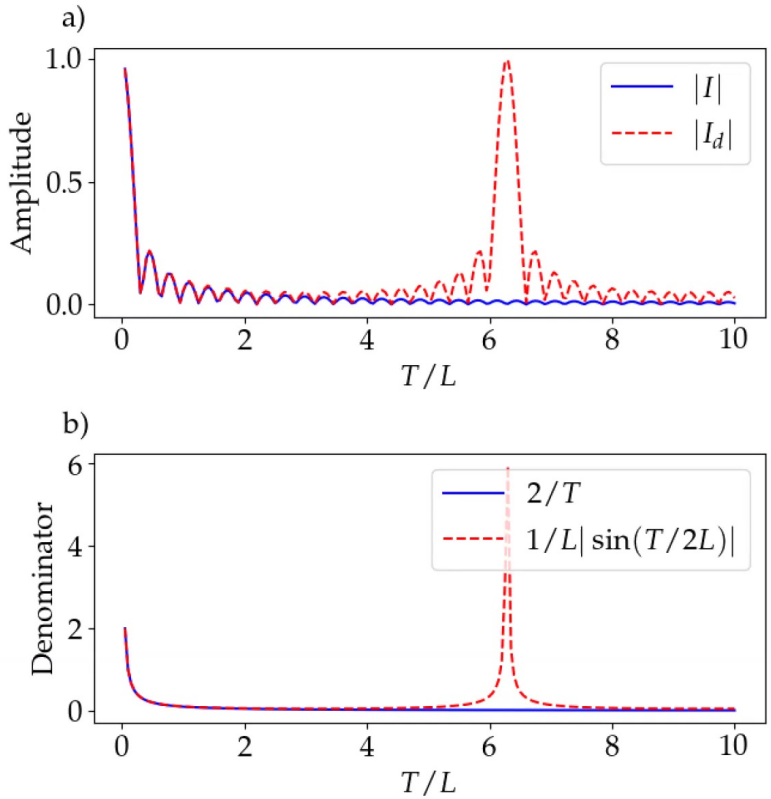
$$I_d = \frac{1}{L}\sum_{k=0}^{L-1} e^{-ikT/L} = \frac{1}{L}\frac{1-e^{-iT}}{1-e^{-iT/L}}, \quad |I_d| = \frac{|\sin(T/2)|}{L|\sin(T/2L)|}$$

Robustness of discrete Riemann-Lebesgue lemma

- When $0 < T/L < 3.78$, we have:

$$\frac{T}{4L} < \sin(\frac{T}{2L}) < \frac{T}{2L}$$

  The impact of discretization is merely a factor of 2
- When $T/L \to 2\pi$, $I_d \xrightarrow{\text{hand}} 1$
- Essentially, this principle accounts for the robustness of DAS



Robustness of discrete Riemann-Lebesgue lemma

- Riemann-Lebesgue lemma

$$I = \int_0^1 f(s)\exp[-iTg(s)]ds, \quad g'(s) > 0, \quad |I| = O\left(\frac{|f(s)|}{T|g'(s)|}\right)$$

- Consider a specific example with $f(s) = 1, g(s) = s$

$$I = \int_0^1 e^{-iTs}ds = \frac{1-e^{-iT}}{iT}, \quad |I| = \frac{|\sin(T/2)|}{T/2}$$

$$I_d = \frac{1}{L}\sum_{k=0}^{L-1} e^{-ikT/L} = \frac{1}{L}\frac{1-e^{-iT}}{1-e^{-iT/L}}, \quad |I_d| = \frac{|\sin(T/2)|}{L|\sin(T/2L)|}$$

Phase error in discrete adiabatic process

- Recall that

$$A_d|0_i\rangle = e^{-i\theta_A}\left(\sqrt{1-\epsilon_{\text{adb}}^2}|0_f\rangle + \sum_{\ell\neq 0}\epsilon_\ell|\ell_f\rangle\right)$$

- The transition rate to higher energy levels ϵ_ℓ allows for large T/L, but the phase error doesn't

$$\delta\theta_A = T\left|\int_0^1 E_0(s)ds - \frac{1}{L}\sum_j E_0(s_j)\right| = O\left(\frac{T}{L}\max_s E_0'(s)\right)$$

- Accordingly, since ϵ_ℓ allows large T/L while $\delta\theta_A$ doesn't, the operator norm distance $\|A - A_d\|$ can be much larger than the fidelity error

Summary

- Numerically, we found the previous upper bound of ϵ_{tot} in DAS overestimates the digital error
- The DAS is a discrete adiabatic process under the effective adiabatic path $\widetilde{H}(s, \delta t)$; so we can apply adiabatic theorem on it as a new estimation
- Analytically, we prove that a large class of discrete adiabatic processes allow large T/L
- As T/L gets larger, eventually the spectral gap of $\widetilde{H}(s, \delta t)$ closes, which results in the breakdown of the robustness, this explains why ϵ_{tot} increases sharply after the critical point. This also means the robustness can break down easily when $\lambda(s)$ is very small
- Q : why does $\langle \ell'(s)|m(s)\rangle$ decrease with $|E_\ell(s) - E_m(s)|$?