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On the complexity of implementing Trotter Steps

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Outline

- **Background**
  - Quantum computing basics
  - Analysis and implementation of Trotter-type formulas
  - Simulation of power-law Hamiltonians
- **Main results**
- **Main techniques**
  - Block encoding and low-rank diagonalization
  - Recursive method and its analysis
  - Quantum simulation in the Hamming weight-2 subspace
- **Summary**

State space

- The state of a single-qubit system is described by ℓ_2-normalized vectors $|\psi\rangle = \beta_0|0\rangle + \beta_1|1\rangle \in \mathbb{C}^2$, with $\{|0\rangle, |1\rangle\}$ orthonormal and $|\beta_0|^2 + |\beta_1|^2 = 1$.
- If two subsystems are in states $|\psi\rangle$ and $|\phi\rangle$ respectively, then the joint system is in the tensor product state $|\psi\rangle \otimes |\phi\rangle$.
- More generally, an n-qubit quantum system can be in state

$$(\mathbb{C}^2)^{\otimes n} \ni \sum_{z_0,\ldots,z_{n-1}=0}^{1} \beta_{z_{n-1},\ldots,z_0} |z_{n-1}\rangle \otimes \cdots \otimes |z_0\rangle$$

$$= \sum_{z_0,\ldots,z_{n-1}=0}^{1} \beta_{z_{n-1},\ldots,z_0} |z_{n-1}, \ldots, z_0\rangle = \sum_{\gamma=0}^{2^n-1} \beta_\gamma |\gamma\rangle \in \mathbb{C}^{2^n}$$

with ℓ_2-normalized coefficients.

Quantum circuit model

- Single-qubit operations are unitaries $U^\dagger U = I$ acting on $\mathbb{C}^2$:

$$X := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad Y := \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad Z := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

$$\mathrm{Had} := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \qquad R_z(\theta) := \begin{bmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{bmatrix}, \qquad T := \begin{bmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix}.$$

- n-qubit operations are unitaries acting on $\mathbb{C}^{2^n}$:

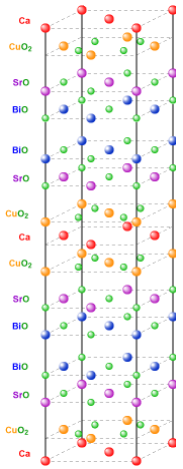
$$\begin{matrix} U \\ V \end{matrix} := U \otimes V, \qquad := \begin{bmatrix} \mathbf{1} & \mathbf{0} & 0 & 0 \\ \mathbf{0} & \mathbf{1} & 0 & 0 \\ 0 & 0 & \mathbf{0} & \mathbf{1} \\ 0 & 0 & \mathbf{1} & \mathbf{0} \end{bmatrix} = |0\rangle\langle 0| \otimes \boldsymbol{I} + |1\rangle\langle 1| \otimes \boldsymbol{X} = |a, b\rangle \xmapsto{\text{CNOT}} |a, b \oplus a\rangle .$$

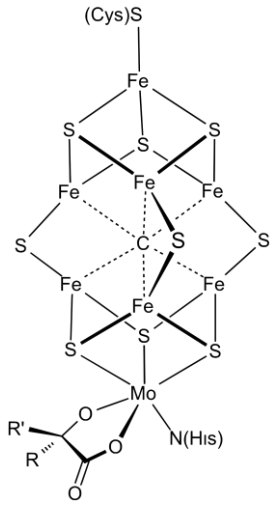
- In the circuit model, quantum computation is realized by a sequence of elementary quantum gates.
- **Complexity** is usually quantified by the **number of gates** that appear in the circuit.

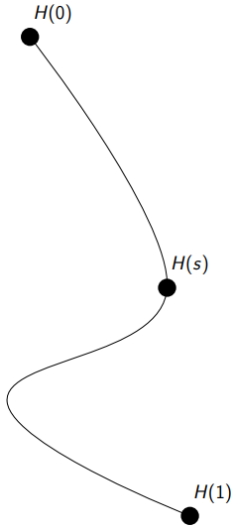
Quantum simulation

Definition: Hamiltonian simulation

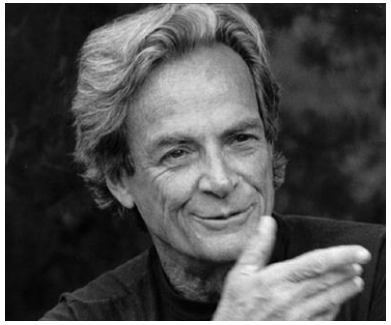
Given a description of Hamiltonian H and evolution time t, approximate e^{-itH} with spectral-norm error $\leq \epsilon$.





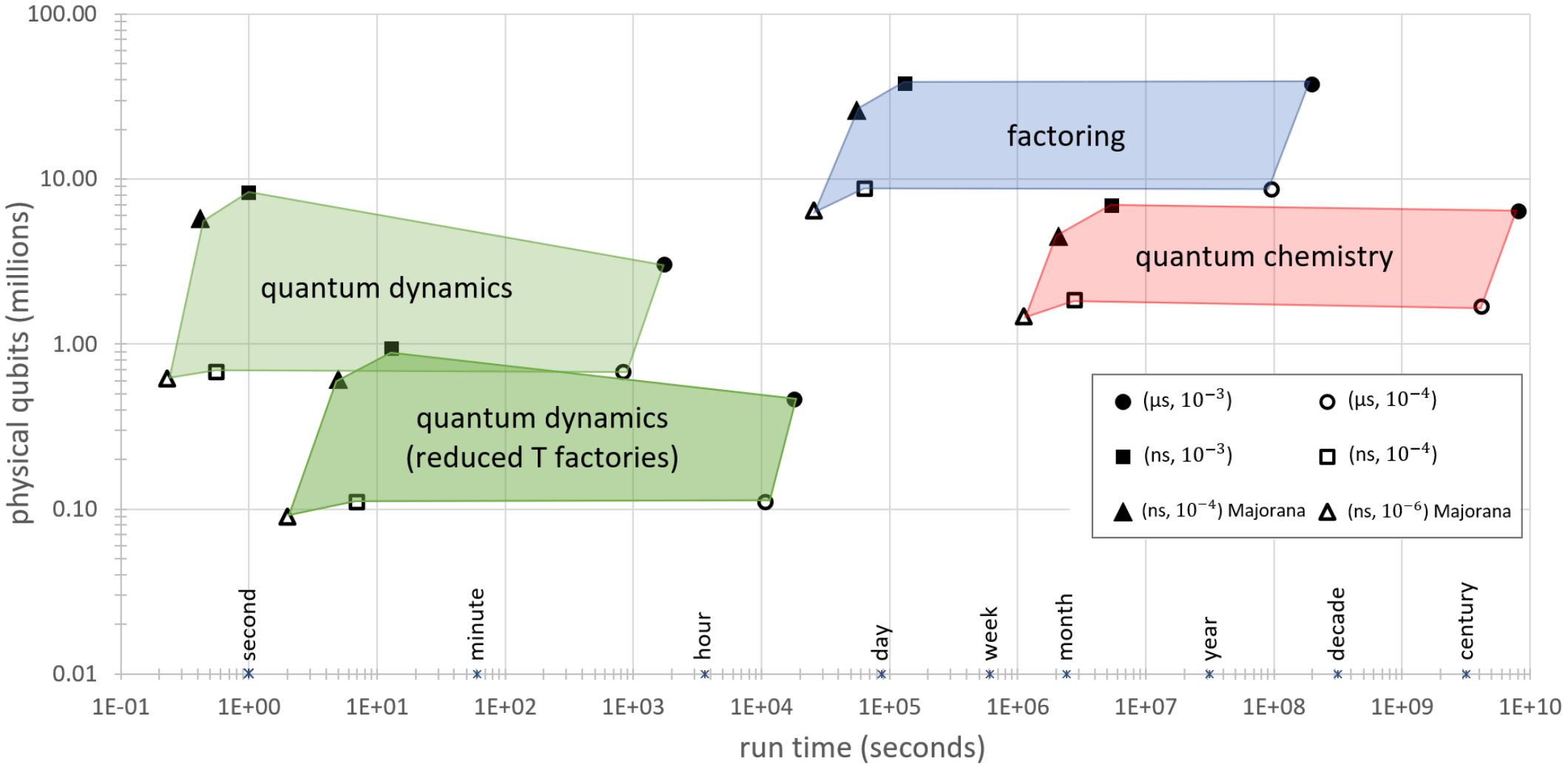


$$A \quad x = b$$



"… nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."

Toward practical quantum advantage



[Beverland, Murali, Troyer, Svore, Hoefler, Kliuchnikov, Low, Soeken, Sundaram, Vaschillo, arXiv:2211.07629]

Trotterization

- Also known as “product-formula method” or “splitting method”.
- Target system: $H = \sum_{\gamma=1}^{\Gamma} H_\gamma$, where each H_γ is Hermitian and can be directly exponentiated on a quantum computer.
- Can use the first-order Lie-Trotter formula

$$S_1(t) := e^{-itH_\Gamma} \cdots e^{-itH_1} = e^{-itH} + \boldsymbol{O(t^2)}$$

  with Trotter error $\boldsymbol{O(t^2)}$.

- Formulas of higher order $S_p(t) = e^{-itH} + O(t^{p+1})$ exist.
- Long-time evolution can be simulated by repeating short steps.
  #Gate = #Step × #Gate/Step.

Trotter error with commutator scaling

- Trotter error has a **commutator scaling**,* which implies commutator scaling of the number of Trotter steps:

$$\#\text{Step} = \mathcal{O}\left(\|\boldsymbol{H}\|_{\boldsymbol{c}} t \left(\frac{\|\boldsymbol{H}\|_{\boldsymbol{c}} t}{\epsilon} \right)^{1/p} \right),$$

$$\|\boldsymbol{H}\|_{\boldsymbol{c}} := \left(\sum_{\boldsymbol{\gamma_1},\ldots,\boldsymbol{\gamma_{p+1}}} \left\| \left[\boldsymbol{H_{\gamma_{p+1}}}, \ldots \left[\boldsymbol{H_{\gamma_2}}, \boldsymbol{H_{\gamma_1}} \right] \right] \right\| \right)^{\boldsymbol{1/(p+1)}}.$$

- One can achieve nearly linear time simulation by using a sufficiently high order formula: $1/p = o(1)$.

* [Childs, Su, Tran, Wiebe, Zhu, arXiv:1912.08854]

Sequential Trotter steps

- Trotter steps can be implemented in a sequential manner.
  But the cost inevitably scales with the total Hamiltonian **term number Γ**.

- For n-qubit 2-local Hamiltonians,

$$\#\text{Gate/Step} \sim \Gamma \sim \binom{n}{2} \sim n^2, \qquad \text{System size} \sim n.$$

- The gap n^κ vs n becomes larger for κ-local systems.

- Can we perform faster Trotter steps with complexity **sublinear in the term number**? When and how?

Power-law Hamiltonians

Definition: 1D Power-law Hamiltonians

$H = \sum_{1 \le j < k \le n} H_{j,k}$, where $H_{j,k}$ are 2-local terms acting nontrivially only on sites j and k with norm $\|H_{j,k}\| \le 1/|j-k|^{\alpha}$ and decay exponent α.

- Many interaction potentials can be expressed as a power-law series

$$v(j,k) = \frac{c_1}{|j-k|} + \frac{c_2}{|j-k|^2} + \frac{c_3}{|j-k|^3} + \cdots$$

- This models physically relevant systems (trapped ions, Rydberg atoms, ultracold atoms/molecules, nitrogen-vacancy centers, and superconducting systems).
- In particular, we improve the electronic structure Hamiltonian simulation in real space ($\alpha = 1$) over the best previous results.

Evaluating commutator scaling

- Terms in the power-law Hamiltonians are nonuniform and satisfy certain commutation relations.
- Cancelling commuting terms, we have

$$\sum_{j_1,k_1,j_2,k_2,j_3,k_3,\ldots,j_{p+1},k_{p+1}} \left\| \left[H_{j_{p+1},k_{p+1}}, \ldots \left[H_{j_3,k_3}, \left[H_{j_2,k_2}, H_{j_1,k_1} \right] \right] \right] \right\|$$

$$= \sum_{\substack{j_1,k_1 \\ j_2 \text{ or } k_2 \in \{j_1,k_1\} \\ j_3 \text{ or } k_3 \in \{j_1,k_1,j_2,k_2\}}} \left\| \left[H_{j_{p+1},k_{p+1}}, \ldots \left[H_{j_3,k_3}, \left[H_{j_2,k_2}, H_{j_1,k_1} \right] \right] \right] \right\|.$$

- Furthermore, for a fixed value of j,

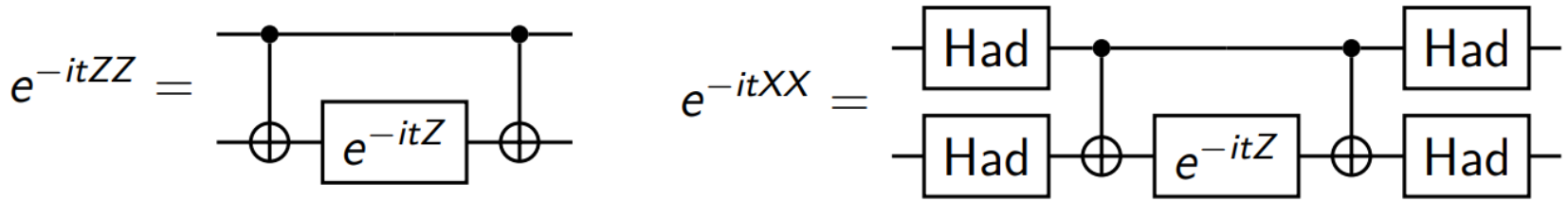
$$\sum_{j<k\leq n} \|H_{j,k}\| \leq \sum_{j<k\leq n} \frac{1}{|j-k|^{\alpha}} = \begin{cases} \mathcal{O}(1), & \alpha > 1, \\ \mathcal{O}(\log n), & \alpha = 1, \\ \mathcal{O}(n^{1-\alpha}), & 1 > \alpha > 0. \end{cases}$$

Exponentiating Pauli strings

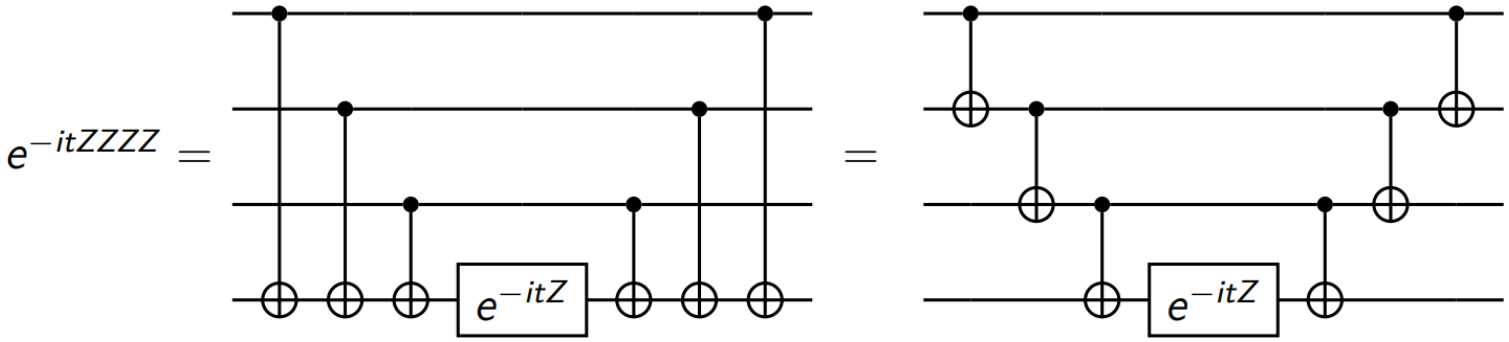
- In the computational basis, ZZ has the action

$$ZZ|00\rangle = |00\rangle, \qquad ZZ|01\rangle = -|01\rangle,$$
$$ZZ|10\rangle = -|10\rangle, \qquad ZZ|11\rangle = |11\rangle.$$

- Exponentiation of Pauli strings can thus be implemented by computing parity (and changing basis):



- Parity trick holds for a general Pauli string:



Best previous result

- For n-qubit 1D power-law Hamiltonians,

$$\#\text{Step} \sim \begin{cases} t(nt/\epsilon)^{o(1)}, & \alpha \geq 1, \\ n^{1-\alpha} t(nt/\epsilon)^{o(1)}, & 1 > \alpha > 0. \end{cases}$$

- Meanwhile, $\#\text{Gate/Step} = \mathcal{O}(n^2)$ with the sequential method.

Method \ Decay	$\alpha \geq 1$	$1 > \alpha > 0$
Sequential*	$n^2 t$	$n^{3-\alpha} t$

Complexity of best previous Trotterization of n-qubit power-law Hamiltonians with decay exponent α for time t and accuracy ϵ, neglecting $(nt/\epsilon)^{o(1)}$ factors.

* [Childs, Su, Tran, Wiebe, Zhu, arXiv:1912.08854]

Our result: Reduced Complexity

- Faster Trotter steps are possible when coefficients in the Hamiltonian have additional structural properties.

Method \ Decay	$\alpha \geq 2$	$2 > \alpha \geq 1$	$1 > \alpha > 0$
Sequential*	$n^2 t$	$n^2 t$	$n^{3-\alpha} t$
Block encoding†	nt	$n^{3-\alpha} t$	$n^{3-\alpha} t$
Average-cost†	—	$n^{2-\alpha/2} t$	$n^{5/2-\alpha} t$
Low-rank†	nt	nt	$n^{2-\alpha} t$

Gate complexity comparison between our Trotterization and the best previous result for n-qubit power-law Hamiltonians with decay exponent α for time t and accuracy ϵ, neglecting $(nt/\epsilon)^{o(1)}$ factors.

* [Childs, Su, Tran, Wiebe, Zhu, arXiv:1912.08854]

† **[Low, Su, Tong, Tran, On the complexity of implementing Trotter steps, arXiv:2211.09133]**

Our result: Application and Limitation

- In **second quantization** in **real space**, Coulomb potential is represented as

$$V \propto \sum_{l,m} \frac{1}{\|l-m\|} N_l N_m = \sum_{l,m} \frac{1}{\|l-m\|} \frac{1-Z_l}{2} \frac{1-Z_m}{2}.$$

- **Application**: With a slightly tighter Trotter error bound, we show that electronic structure can be simulated with gate complexity

$$\left(\frac{\eta^{2/3} n^{4/3}}{\omega^{1/3}} + \frac{n^{5/3}}{\omega^{2/3}} \right) \frac{n^{o(1)} t^{1+o(1)}}{\epsilon^{o(1)}},$$

  with $\eta =$ #electrons and $\omega =$ the computational cell volume, giving the **fastest simulation of electronic structure Hamiltonians in real space**.

- Limitation: **sequential method is optimal if Hamiltonian coefficients take arbitrary values**.

Block encoding as unitary dilation

- Problem: given matrix H, construct a unitary U such that

$$U = \begin{bmatrix} H & * \\ * & * \end{bmatrix}.$$

- This unitary dilation is mathematically feasible if and only if $\|H\| \leq 1$: if $H = V\Sigma W^\dagger$ is SVD, then define

$$U = \begin{bmatrix} V & 0 \\ 0 & V \end{bmatrix} \begin{bmatrix} \Sigma & -\sqrt{1-\Sigma^2} \\ \sqrt{1-\Sigma^2} & \Sigma \end{bmatrix} \begin{bmatrix} W^\dagger & 0 \\ 0 & W^\dagger \end{bmatrix}.$$

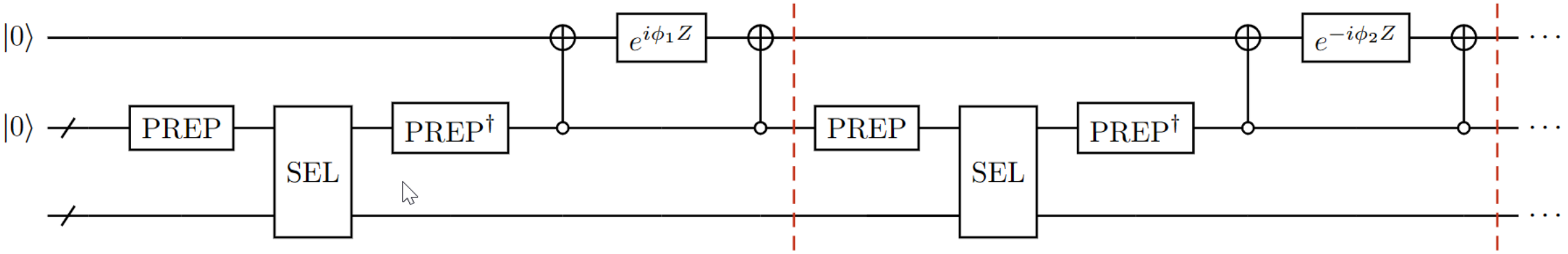
- Assume $H = \sum_{\gamma=1}^{\Gamma} \beta_\gamma U_\gamma$, where $\beta_\gamma > 0$ and U_γ are Hermitian unitaries such that $|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U_\gamma$ can be directly implemented. Then choosing

$$\mathrm{PREP}|0\rangle = \frac{1}{\sqrt{\|H\|_1}} \sum_{\gamma=1}^{\Gamma} \sqrt{\beta_\gamma}|\gamma\rangle, \quad \mathrm{SEL} = \sum_{\gamma=1}^{\Gamma} |\gamma\rangle\langle\gamma| \otimes U_\gamma$$

gives $\left(\langle 0|\mathrm{PREP}^\dagger \otimes I\right)\mathrm{SEL}(\mathrm{PREP}|0\rangle \otimes I) = \frac{H}{\|H\|_1}$ with $\|H\|_1 = \sum_\gamma \beta_\gamma$.

Block encoding & quantum simulation

- One can perform quantum simulation by introducing auxiliary qubits and **running quantum algorithms on larger Hilbert spaces**.
- Assume $H = \sum_{\gamma=1}^{\Gamma} \beta_\gamma U_\gamma$, where $\beta_\gamma > 0$ and U_γ are Hermitian unitaries such that $|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U_\gamma$ can be directly implemented.
- Then, perform the following circuit #Step $\sim \|\boldsymbol{H}\|_1 t = (\sum_\gamma \boldsymbol{\beta_\gamma}) t$



where $\mathrm{PREP}|0\rangle = \frac{1}{\sqrt{\|H\|_1}} \sum_{\gamma=1}^{\Gamma} \sqrt{\beta_\gamma}|\gamma\rangle$, $\mathrm{SEL} = \sum_{\gamma=1}^{\Gamma} |\gamma\rangle\langle\gamma| \otimes U_\gamma$.*

* [Low, Chuang, arXiv:1610.06546]

Block encoding cost

- SEL has cost often **linear in the system size**:

$$\mathrm{SEL}=\sum_{u,v=1}^{n}|u,v\rangle\langle u,v|\otimes X_u Y_v=\left(\sum_{u=1}^{n}|u\rangle\langle u|\otimes X_u\right)\left(\sum_{v=1}^{n}|v\rangle\langle v|\otimes Y_v\right),$$

  PREP can be improved correspondingly using structural properties of the coefficients. So **#Gate/Step $\sim \boldsymbol{n}$**.

- However, unlike Trotter, qubitization does not have a commutator scaling

$$\#\mathrm{Step}\sim \|\boldsymbol{H}\|_1 t=\left(\sum_{\boldsymbol{\gamma}}\boldsymbol{\beta}_{\boldsymbol{\gamma}}\right)t,$$

  which completely washes out the improvements from PREP and SEL for power-law interactions.

Low-rank diagonalization

- For a Hamiltonian with commuting terms, quantum simulation can be realized using a diagonalization circuit.
- Suppose $H = \sum_{u,v} \beta_{u,v} Z_u Z_v$ and the coefficient tensor has a singular value decomposition with rank ρ

$$\beta_{u,v} = \sum_{s=1}^{\rho} \mu_{u,s} \sigma_s \nu_{v,s} .$$

- Then we can simply compute the diagonal phase factors

$$e^{-itH} |z_n, \dots, z_1\rangle = e^{-it\sum_{s=1}^{\rho} \sigma_s \left(\sum_u \mu_{u,s} (-1)^{z_u}\right)\left(\sum_v \nu_{v,s} (-1)^{z_v}\right)} |z_n, \dots, z_1\rangle$$

with cost $\sim \rho n$ depending on the rank.

- However, the coefficient tensor of a general power-law Hamiltonian does not have low rank.

Recursion & the master theorem

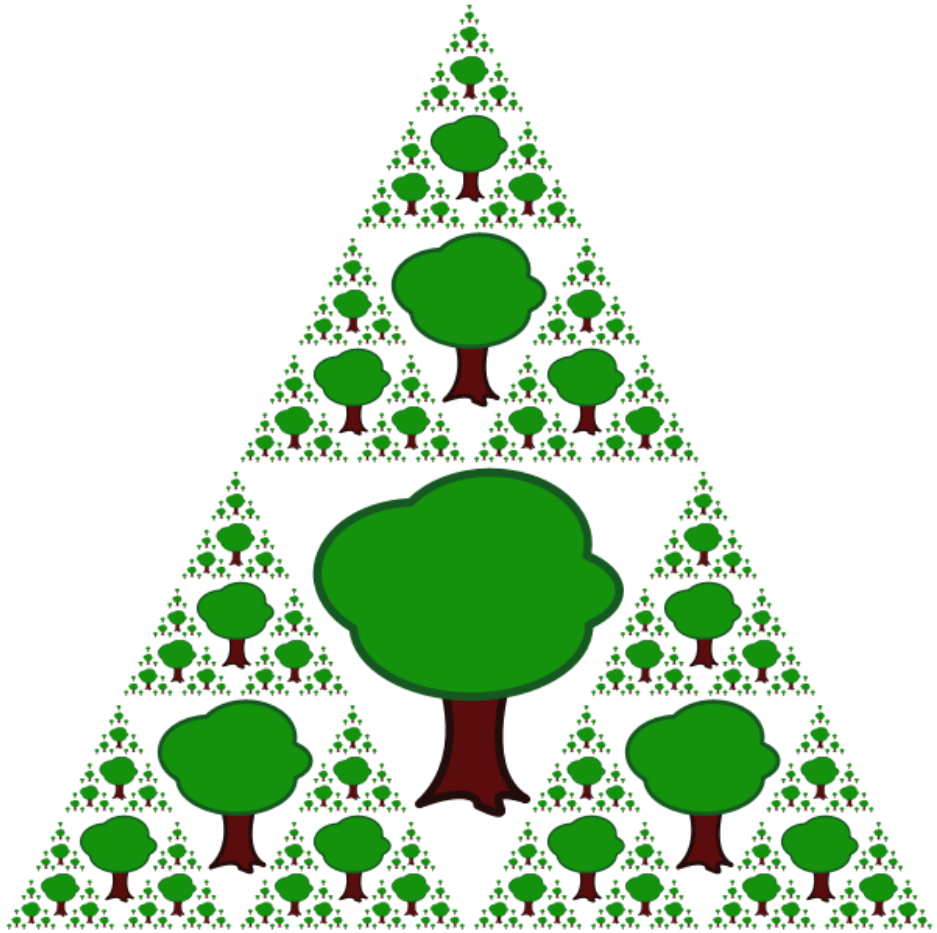
- Solve a problem of size n by **solving m subproblems, each of size n/m, and combining the answers**.

- The complexity of recursion can be obtained from the master theorem:*

$$\text{cost}_{\text{rec}}(n) = m \cdot \text{cost}_{\text{rec}}\left(\frac{n}{m}\right) + \text{cost}(n)$$

$$\Downarrow$$

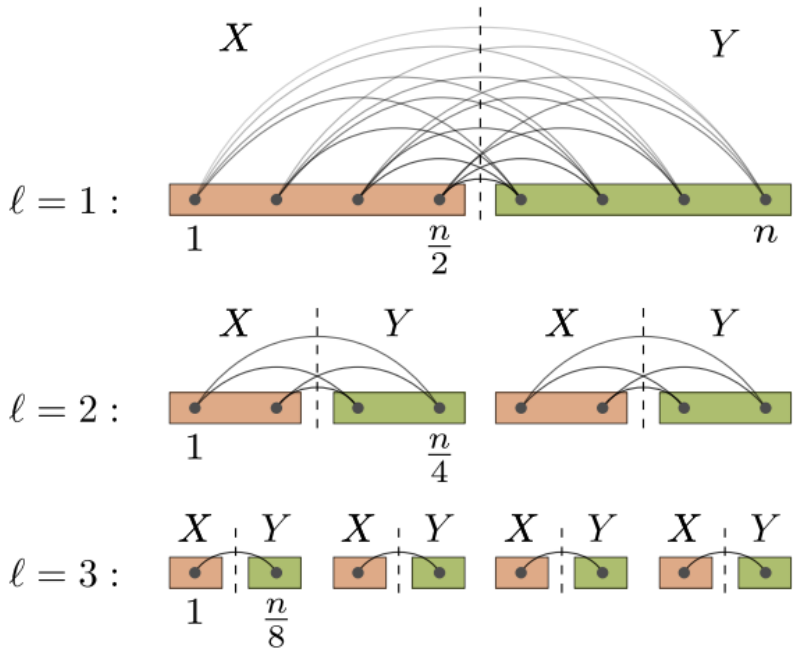
$$\mathbf{cost_{rec}}(n) = \mathcal{O}(\mathbf{cost}(n)\log(n) + n)$$

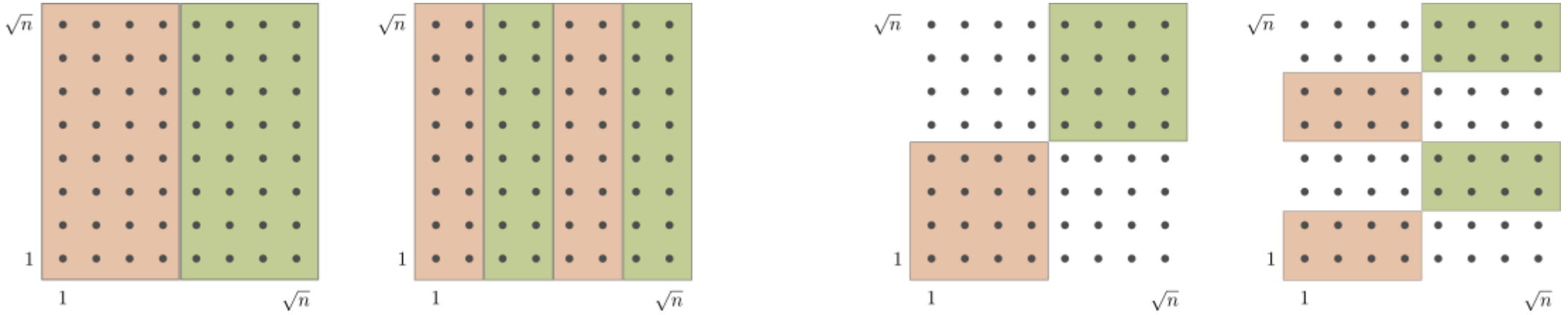


* [CLRS, Introduction to Algorithms '22] [Neapolitan, Foundations of Algorithms '14]

Recursive block encoding

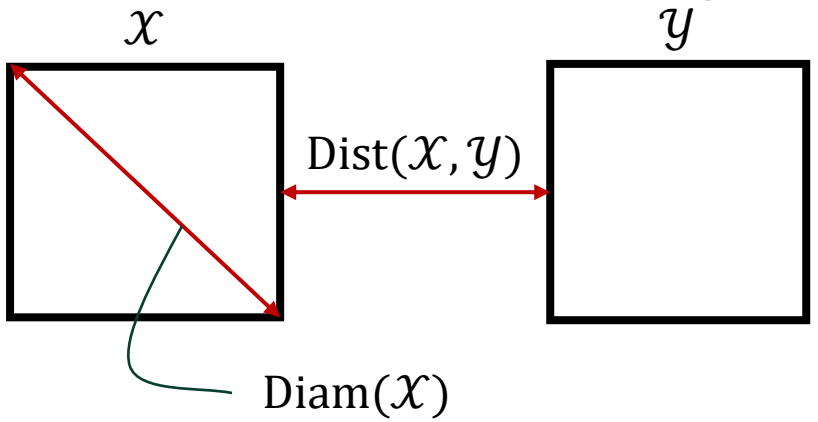
- With a suitable recursion, the number of qubitization steps regains the commutator scaling of Trotterization.
- This can be further improved for small α by simulating commuting terms with an average combination cost.





Analysis of Taylor approximation

- Power function $f(x,y) = \frac{1}{\|x-y\|^{\alpha}}$ can be uniformly Taylor approximated, with error determined by size and distance of the regions f acts on.



- Specifically, truncating the Taylor series of d-dimensional power functions at order m gives*

$$\text{error: } \left\|f-\tilde{f}\right\|_{\max,\mathcal{X}\times\mathcal{Y}} = \mathcal{O}\left(\left(\frac{c\,\mathrm{Diam}(\mathcal{X})}{\mathrm{Dist}(\mathcal{X},\mathcal{Y})}\right)^{m}\right), \qquad \text{rank: } \rho = \mathcal{O}\left(m^{d}\right),$$

where constant $c > 1/2$ can be chosen arbitrarily close to ½.

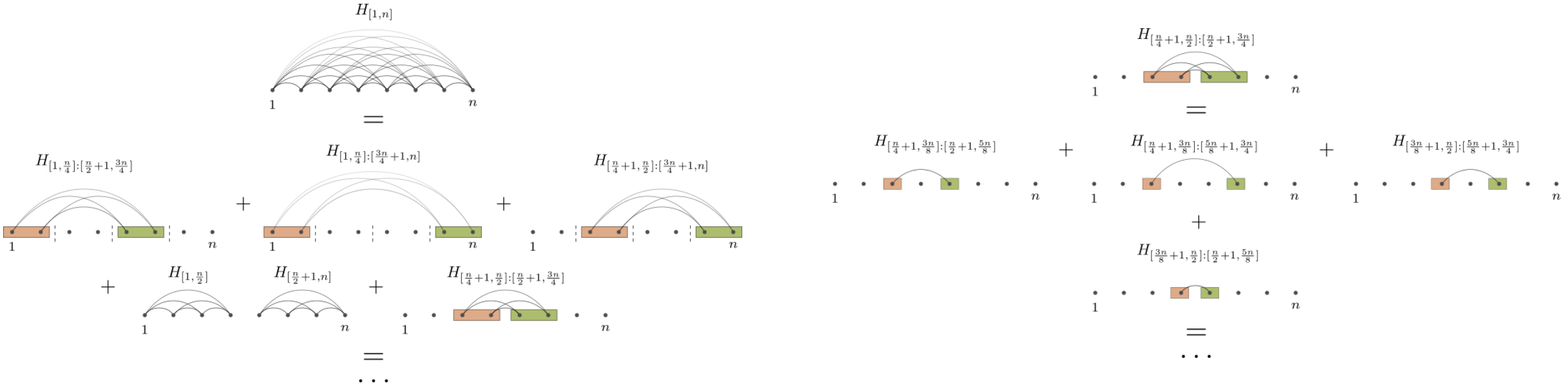
*[Hackbusch, Hierarchical Matrices: Algorithms and Analysis '15, Theorem 4.22]

Recursive low-rank method

- Using the division-by-half strategy, we have

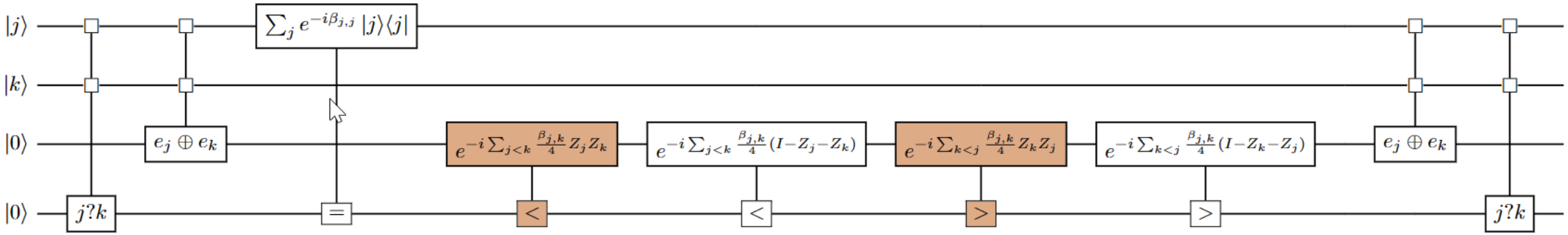
Dimensions	$d = 1$	$d = 2$	$d = 3$
$\frac{c\,\mathrm{Diam}(\mathcal{X})}{\mathrm{Dist}(\mathcal{X},\mathcal{Y})}$	$\approx \frac{1}{2} = 0.5$	$\approx \frac{\sqrt{2}}{2} = 0.707\ldots$	$\approx \frac{\sqrt{3}}{2} = 0.866\ldots$

Thus, the Taylor error decays exponentially with the truncate order m.



Simulation in Hamming weight-2 subspace

- If coefficients of a 2-local Hamiltonian have no specific structure, then one needs $\Omega(n^2)$ gates to simulate with $\epsilon = \Omega(1/\mathrm{poly}(n))$ for $t = \Omega(\epsilon)$.
- We give a gate-efficient reduction: **performing diagonal unitaries** can be accomplished by **simulating 2-local commuting Hamiltonians** in the Hamming weight-2 subspace.



- Lower bound then follows from a volume-comparison technique.*

*[Knill, arXiv:quant-ph/9508006]

Summary

- We develop recursive methods to perform Trotter steps using structures of Hamiltonian coefficients, going beyond the sequential approach.
- #Gate/Step is sublinear in the Hamiltonian term number, while #Step still maintains the commutator scaling.
- The new result gives the fastest quantum simulation of second-quantized electronic structure Hamiltonians in real space. Further studies on first-quantized quantum simulation could be interesting.
- However, Trotter steps are hard to asymptotically improve if Hamiltonian coefficients are arbitrarily chosen.
- It could be fruitful to further optimize Trotter circuits and error bounds, or to find applications of product formulas beyond quantum simulation.

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"On the complexity of implementing Trotter Steps"
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