Microsoft

arXiv:1801.03922

with Hastings, Kothari, Low

Quantum algorithm for simulating real time evolution of lattice Hamiltonians

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Hamiltonian Simulation

"...If you want to make a simulation of nature,
you'd better make it quantum mechanical."

– R. Feynman

- Condensed matter/high energy/AMO physics
- Quantum chemistry
- Linear equation solver
- Optimization as ground state finding

Conceptually, it is manifestation of determinism in physics.

Problem

Input: a local Hamiltonian $H = \sum_X h_X$

(NOT “low-weight” Hamiltonian as in Hamiltonian complexity theory)

Output: Time-evolution unitary $U_t^H = \mathbf{exp}(-itH)$

- H is huge as a matrix; $\mathbf{exp}(V)$.
- Output = $poly(V, t)$ elementary gates
- Sufficient to produce $U \simeq U_t^H$ to accuracy ϵ in operator norm

Previous algorithms

- "Infinitesimal time evolutions commute."
  - $e^{-it(A+B)} \simeq \left(e^{-\frac{itA}{n}} e^{-\frac{itB}{n}}\right)^n$ (Lloyd 1996)
  - Higher order (randomized) Suzuki: $V(VT)^{1+\frac{1}{(2)k}}/\epsilon^{\frac{1}{(2)k}}$ (Childs et al. 2017)
  - For local interactions it was claimed that $(VT)^{1+\frac{1}{k}}/\epsilon^{\frac{1}{k}}$ gates suffice. (Jordan-Lee-Preskill 2014)
- For sparse Hermitian $2^n \times 2^n$ matrices:
  - Taylor series: $\tilde{O}\left(n^2 T \log\frac{1}{\epsilon}\right)$
  - Quantum signal processing: $\tilde{O}\left(n^2 T + n \log\frac{1}{\epsilon}\right)$

Our Result

For any bounded local (time-independent) Hamiltonian on Euclidean lattices, we can write a quantum circuit $\boldsymbol{U}$ of depth $\boldsymbol{O}\left(t \log^{\alpha}\left(\frac{tV}{\epsilon}\right)\right)$ and total gate count $\boldsymbol{O}\left(tV \log^{\alpha}\left(\frac{tV}{\epsilon}\right)\right)$ such that $\left\|U - U_t^H\right\| \leq \epsilon$ for a const $\boldsymbol{\alpha} > \mathbf{0}$.

For time-dependent case, we need $\boldsymbol{H}$ be slowly varying and each term must be efficiently computable.

Lieb-Robinson Bounds

$$\simeq$$

Quantum Circuit Decomposition

Absolute Lightcone even in nonrelativistic systems

Lieb-Robinson 1972
Hastings, Koma 2004,2006
Nachtergaele-Sims 2006
Premont-Schwarz et al. 2010

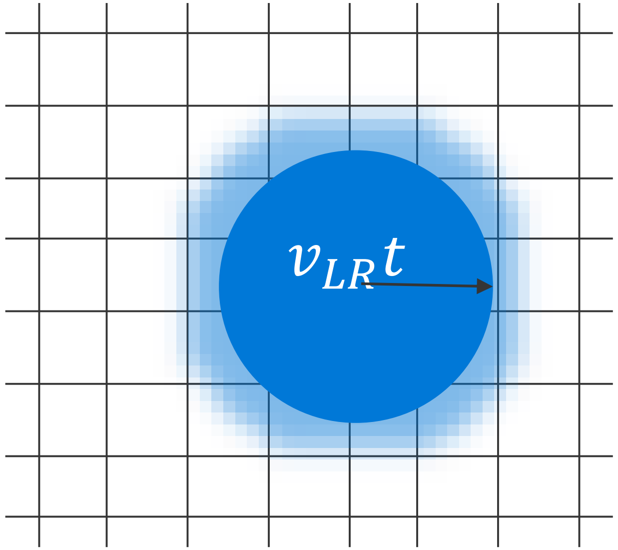
- $A_X(t) = e^{itH} A_X e^{-itH}$ acts everywhere once $t > 0$, but not substantially everywhere.

$$|| [A_X(t), B_Y] || \le 2|X| \frac{(\zeta t)^\ell}{\ell!} \text{ where } \ell = dist(X,Y)$$

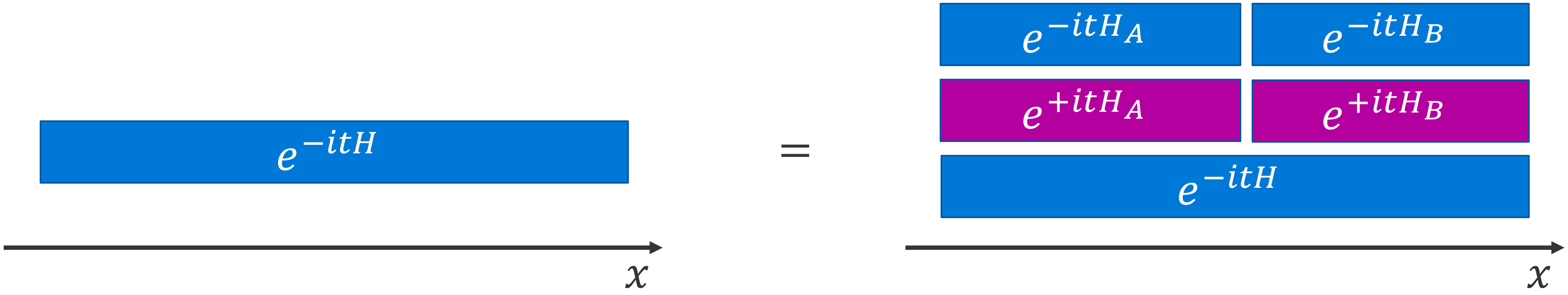
$$H_\Omega = \sum_{X \subseteq \Omega} h_X$$

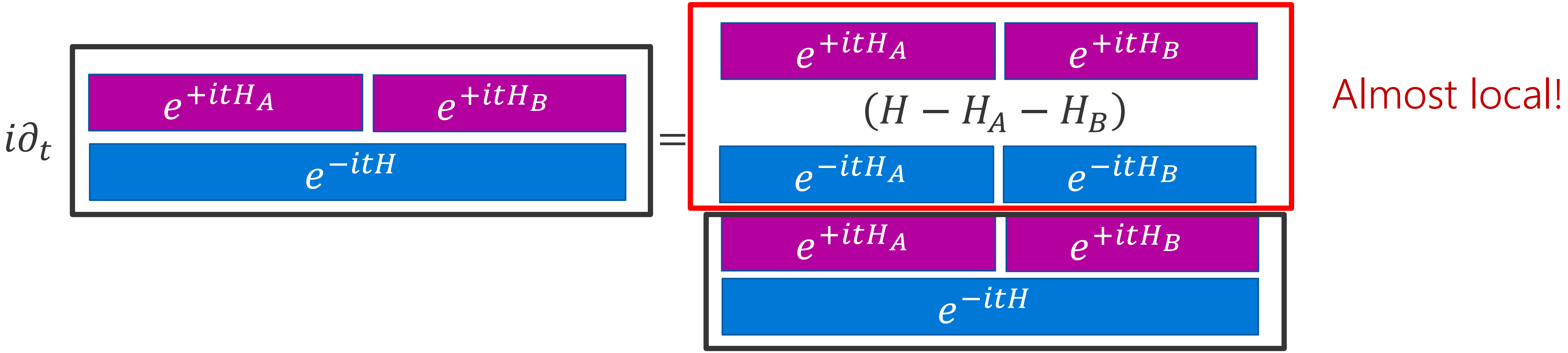
$$|| A_X(t;H) - A_X(t;H_\Omega) || \le |X| \frac{(\zeta t)^\ell}{\ell!} \text{ where } \ell = dist(X,\Omega^c)$$

- Independent of interaction detail, but only locality and strength (ζ).
- Holds not only for lattices, but also for bounded degree graphs.



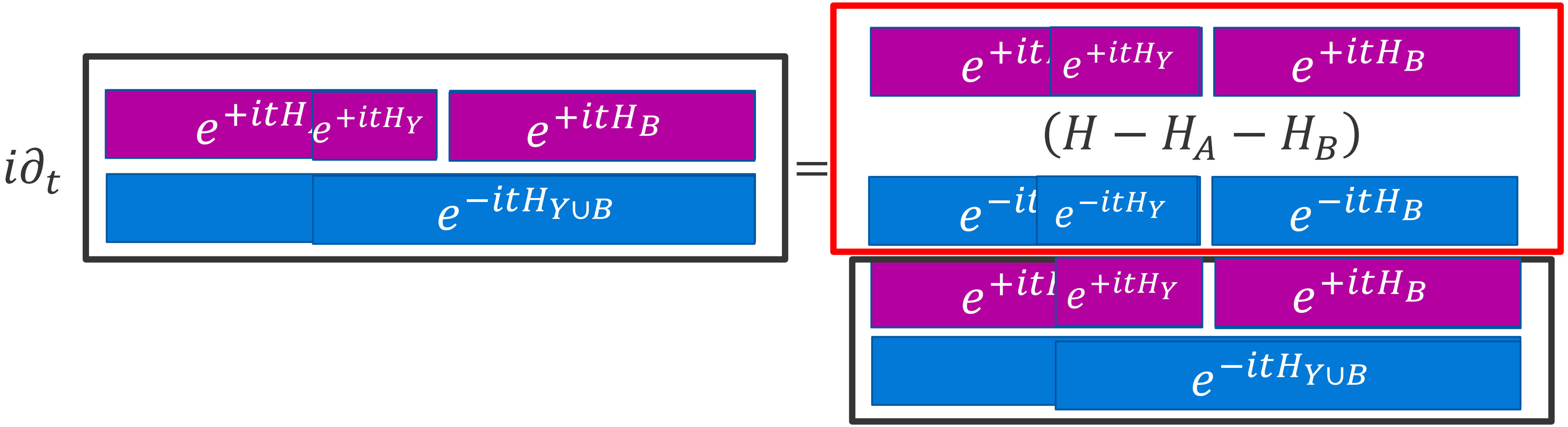
Curing Naïve Decomposition (Osborne 2006)



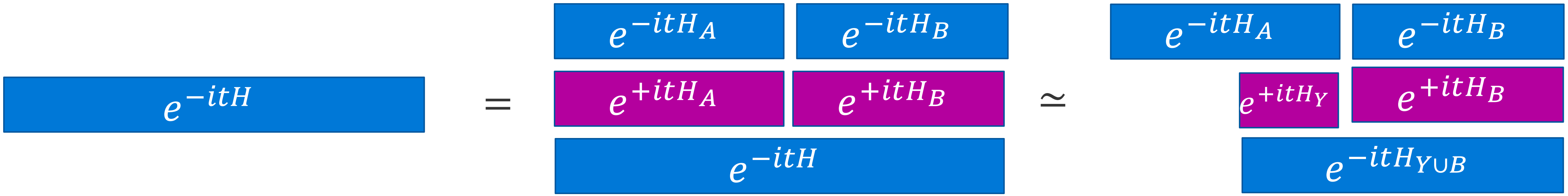


Schroedinger equation by an almost local Hamiltonian.

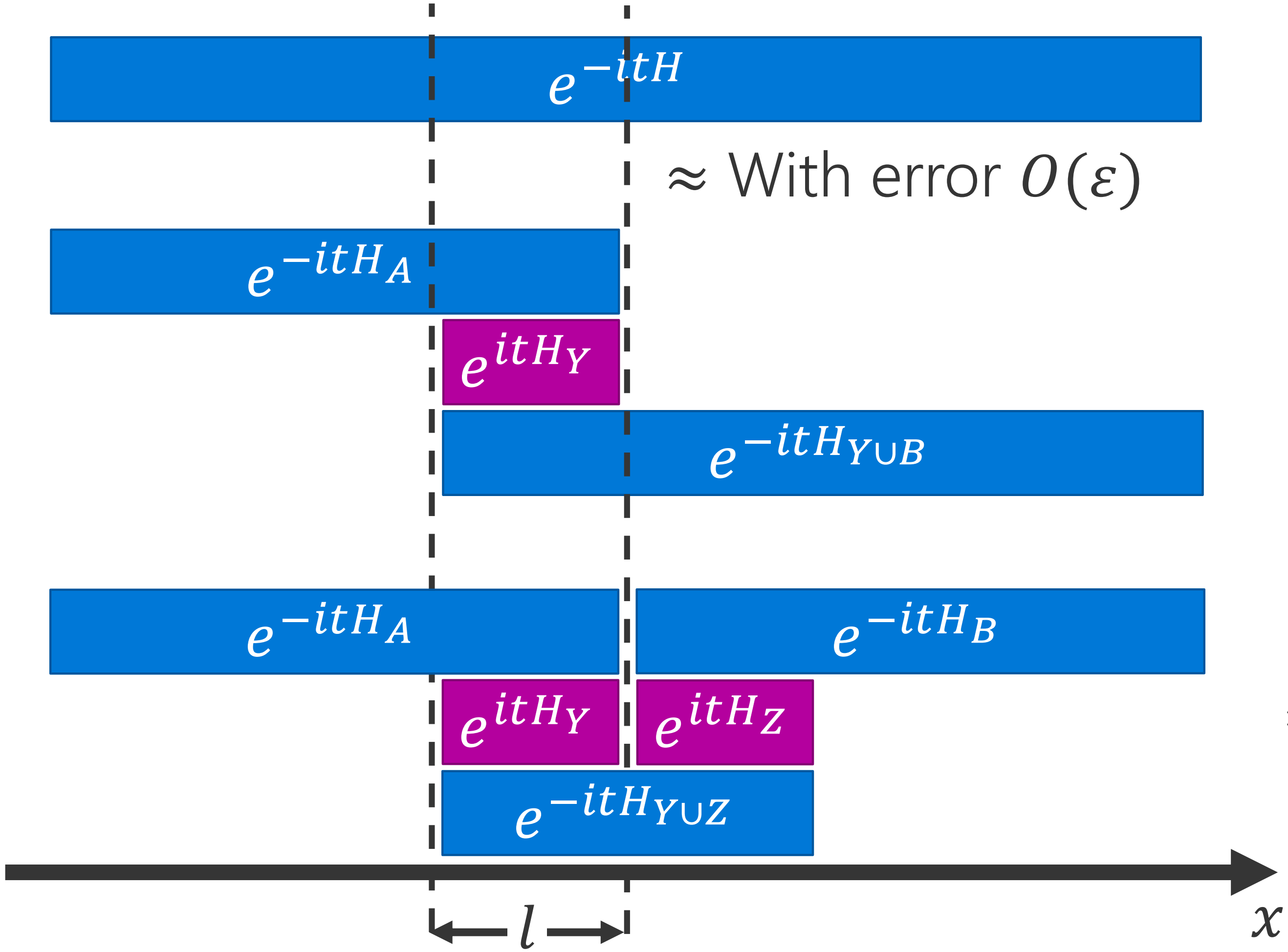
Further Simplification



$$|| A_X(t;H) - A_X(t;H_\Omega)|| \leq |X| \frac{(\zeta t)^\ell}{\ell!} \text{ where } \ell = dist(X, \Omega^c)$$



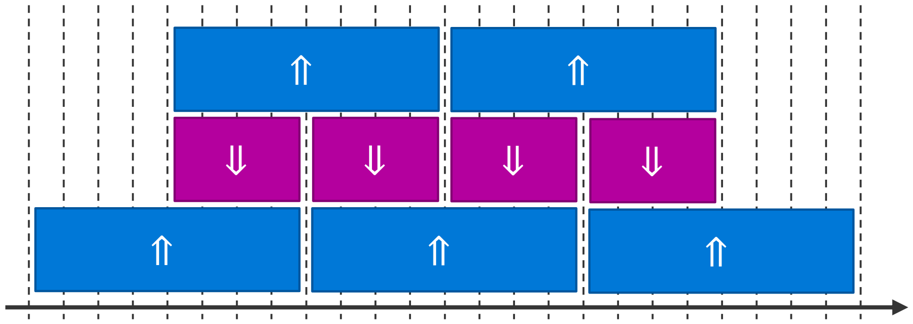
Iterative Decomposition



We choose $t = 1$

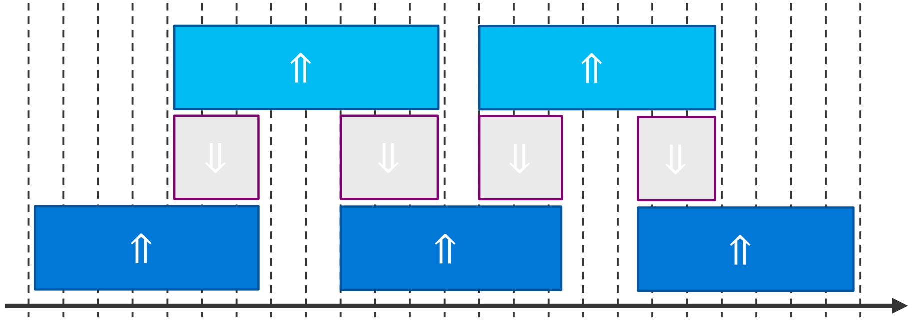
$$l = O(vt + \log(1/\varepsilon))$$

$\approx$



Higher dimensions

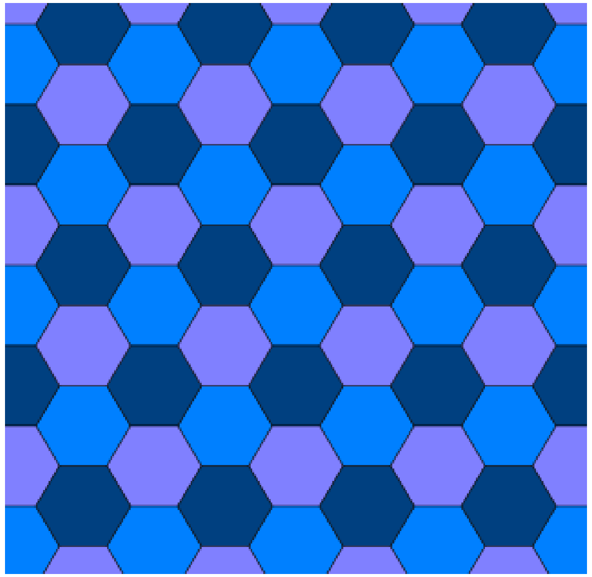
2-colorable



+ Color 1
- Color 1 ∩ 2
+ Color 2

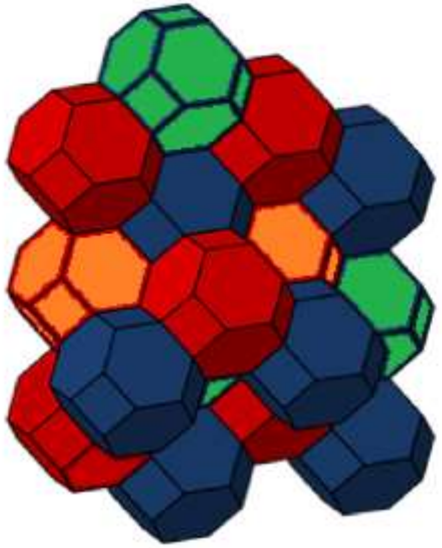
$2\alpha - 1$ layers per unit time

3-colorable



+ Color 1
- Color 1 ∩ 2
+ Color 2
- Color (1 ∪ 2) ∩ 3
+ Color 3

4-colorable

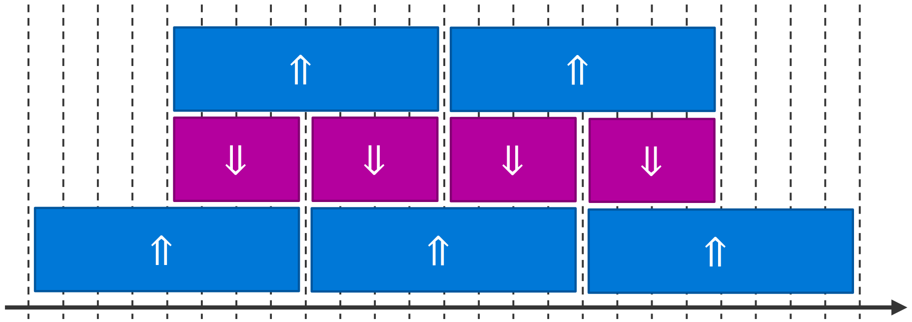


+ Color 1
- Color 1 ∩ 2
+ Color 2
- Color (1 ∪ 2) ∩ 3

…….

Implementing small blocks

- Requirements
  - Block size ~ Overlap size $\ell = O(vt + \log(1/\varepsilon_{LR}))$
    (we take $t = 1$ and repeat T times.)
  - #(Blocks) $< VT$. It suffices to have $\epsilon_{LR} < \frac{\epsilon}{VT}$.
  - $\ell = O\left(\log\left(\frac{VT}{\epsilon}\right)\right)$
  - Each block has to be good to $\epsilon_{\blacksquare} < \epsilon / VT$.



- Full gate count =
  #(Lieb-Robinson blocks) × cost[size $\mathbf{log}(\frac{\boldsymbol{VT}}{\boldsymbol{\epsilon}})$, accuracy $\frac{\boldsymbol{\epsilon}}{\boldsymbol{VT}}$]
- Already we have $\boldsymbol{poly}\left(\ell, \log\left(\frac{1}{\epsilon}\right)\right)$ algorithms.

Linear combination of unitaries

Childs-Wiebe 2012,
Berry et al. 2014

$$U = \alpha_1 U_1 + \alpha_2 U_2 + \cdots + \alpha_n U_n$$

1. Prepare: $B|0\rangle = |\alpha\rangle \propto \sum_j \sqrt{\alpha_j}\, |j\rangle$ on ancilla.
2. Implement $\sum_j |j\rangle\langle j| \otimes U_j$
3. Apply B^{-1}.
4. Measure the ancilla, abort if nonzero.
5. Success probability can be boosted.

- A Hamiltonian is a linear combination of $O(V)$ unitaries.
- So is $e^{-itH} \simeq \sum_{k=0}^{K} \frac{(-itH)^k}{k!}$.

Quantum signal processing (Low-Chuang 2016)

$H = \alpha_1 U_1 + \alpha_2 U_2 + \cdots + \alpha_n U_n$

can be inferred from a unitary

$$(2|\alpha\rangle\langle\alpha| - 1)\left(\sum_j |j\rangle\langle j| \otimes U_j\right)$$

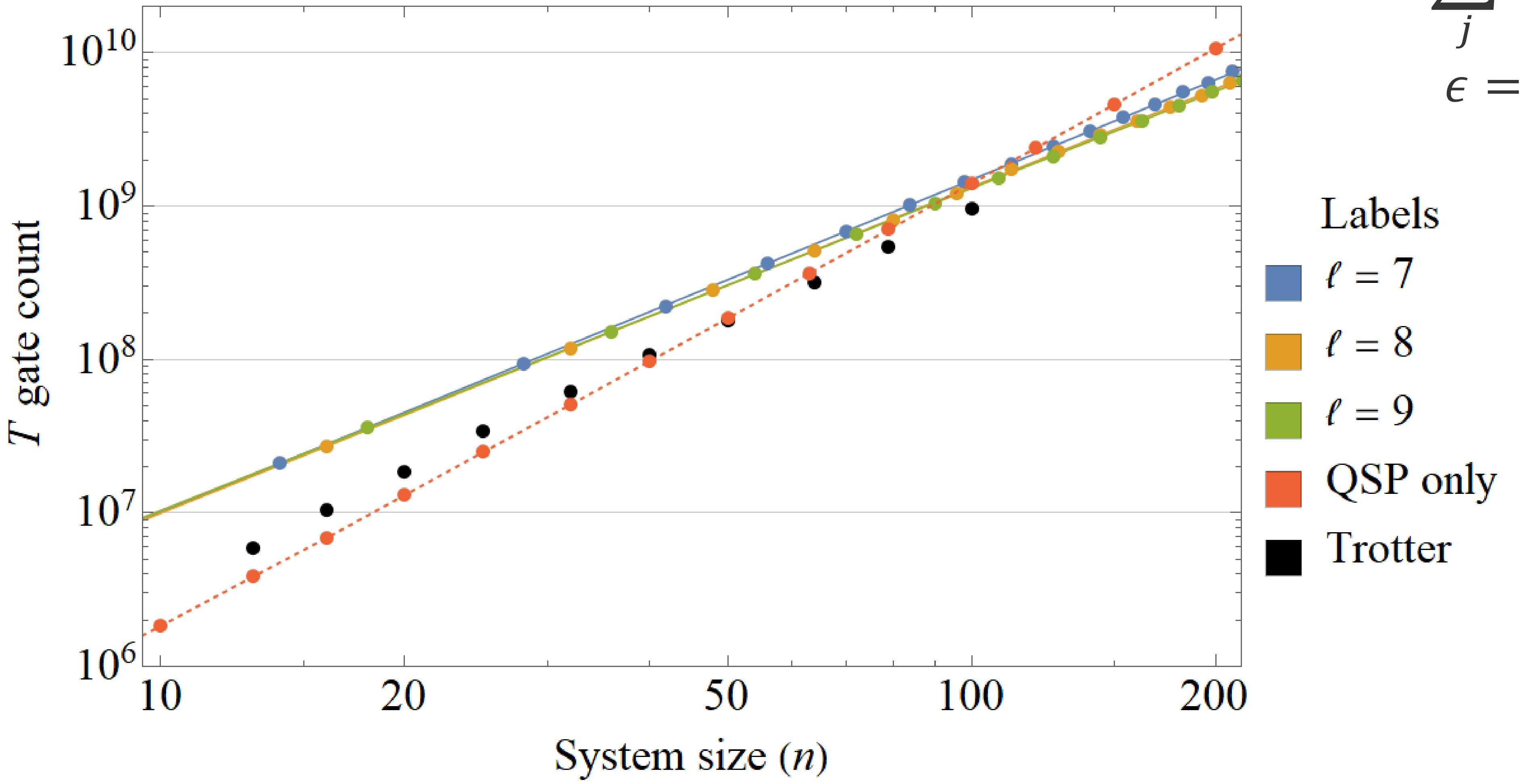
- QSP: $\sum_a \lambda_a |a\rangle\langle a| \mapsto \sum_a f(\lambda_a) |a\rangle\langle a|$
- Much fewer ancilla qubits than Taylor series approach
- Lower gate count $\tilde{O}\left(n^2 T + n \log \frac{1}{\epsilon}\right)$
- Unsure how to use for time-dependent Hamiltonians

Gate count estimates

Microsoft Quantum Development Kit
http://www.Microsoft.com/quantum

$$H = \sum_j \vec{\sigma}_j \cdot \vec{\sigma}_{j+1} + \sum_j h_j \sigma_j^z$$

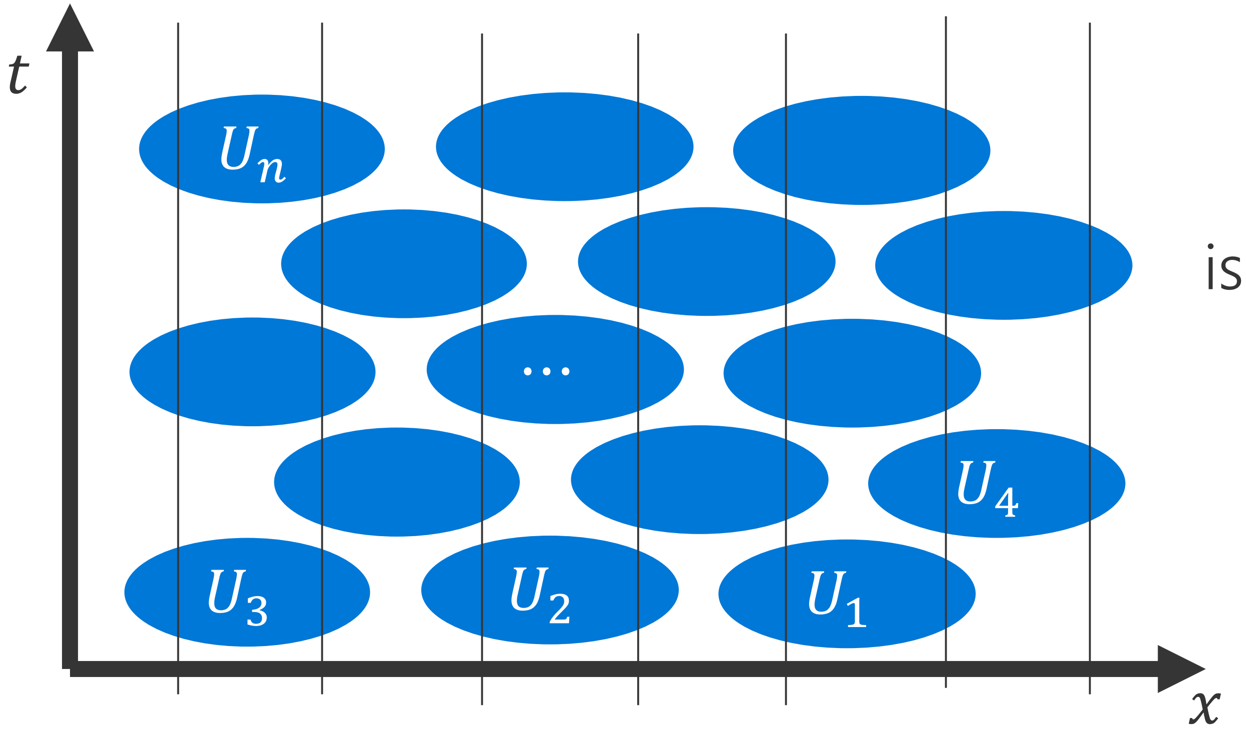
$$\epsilon = 10^{-3},\ T = n$$



Optimality:

Any general algorithm must have $\widetilde{\Omega}(VT)$ gates.

Any circuit is time-evolution

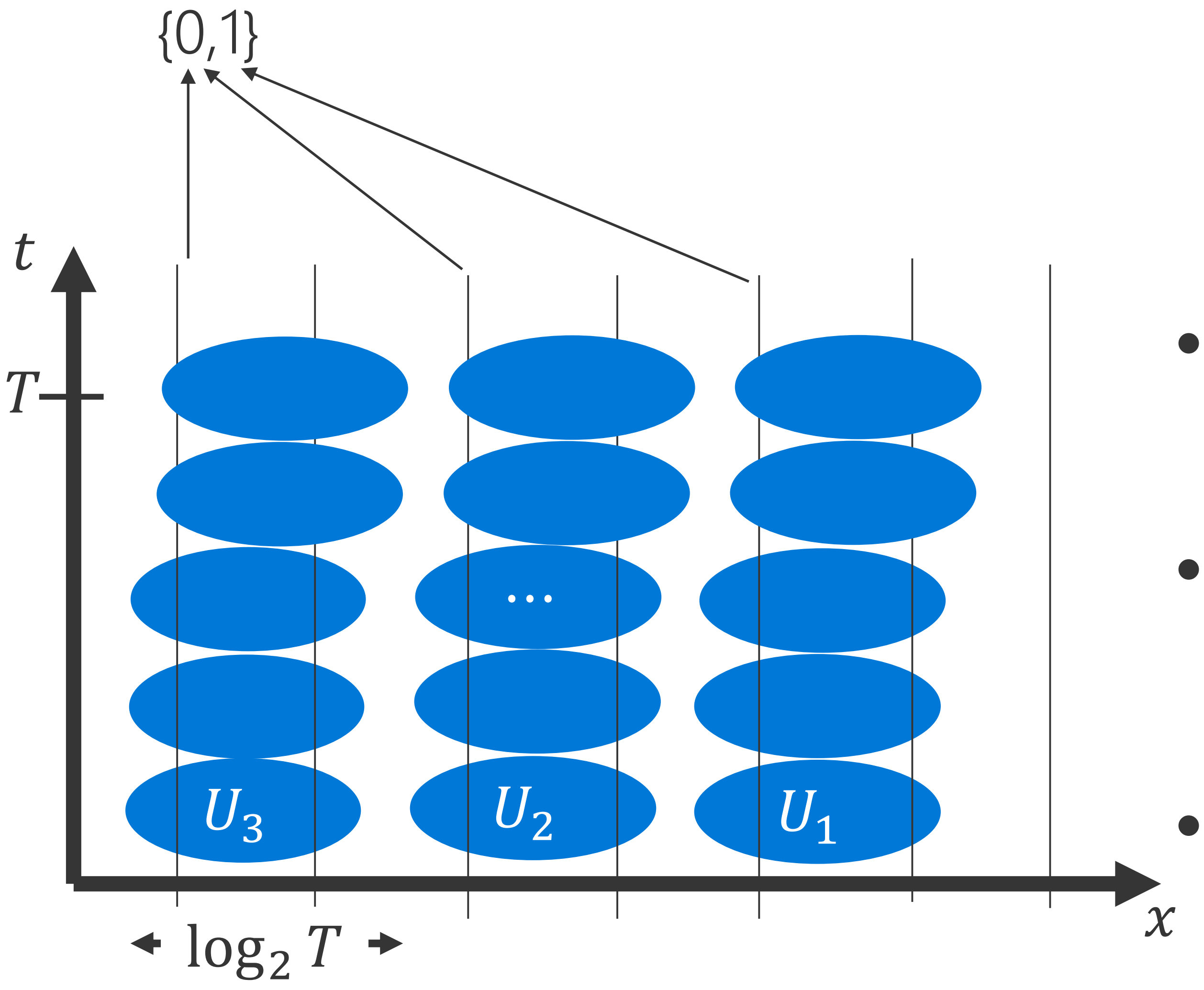


$$U_5 = \exp(-i \cdot \boldsymbol{i \log(U_5)})$$

is the exponential of a local Hermitian operator

- Any quantum circuit is the time-evolution of a piecewise constant (time-dependent) local Hamiltonian

How expressive is a circuit?



- In each column of $\mathbf{k} = \log_2 T$ qubits any $f: \{0,1\}^k \to \{0,1\}$ can be computed.
- There are $2^{2^k} = 2^T$ such functions.
- Thus, $2^{TV/\log_2 T}$ maps can be expressed.
- $\exp\left(\widetilde{\Omega}(TV)\right)$, even if we turn it into a $\{0,1\}$-valued function.

Argument combined

- Depth-T circuits on V qubits can express $\exp(\widetilde{\Omega}(TV))$ Boolean functions.
- A general Hamiltonian simulation algorithm for time T can implement every such function.
- G quantum gates can only express $2^{\tilde{O}(G)}$ different functions.

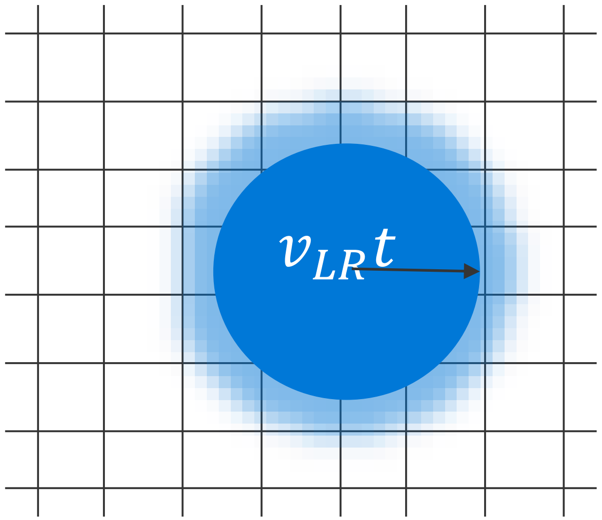
$$G = \widetilde{\Omega}(TV)$$

Even if we care a local observable only.

Bonus:
Lieb-Robinson bound for (un)bounded H

- $H = \sum_X h_X$ such that $\left|\left|h_X\right|\right| < \infty$ and $\left|\left|[h_X, h_Y]\right|\right| \leq K$
- Then,

$$|| A_X(t; H) - A_X(t; H_\Omega)|| \leq |X| \frac{(\zeta t\sqrt{K})^\ell}{\ell!}$$

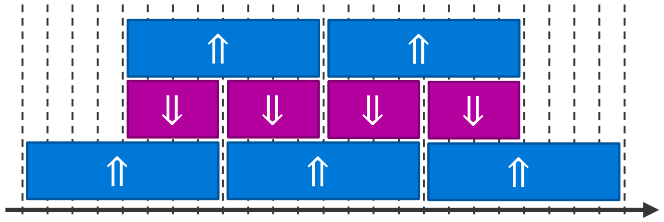


where $\ell = dist(X, \Omega^c)$

Previously, H had to consist of two "terms."
(Premont-Schwarz et al. 2010)

Local Hamiltonian simulation is as efficient as possible.

- Local interaction limits speed of correlation propagation.



- Lieb-Robinson bounds give a natural decomposition of time-evolution unitary into $\mathbf{log}(VT/\epsilon)$-sized blocks.
- Each block is again a Hamiltonian time-evolution with $\boldsymbol{polylog}(VT/\epsilon)$ alg.
- Covers fermion.
- Gate complexity $\tilde{O}(VT)$ is optimal, because time-evolution is expressive.
- Algorithms for low energy sectors…?