3. Hamiltonian Simulation: Basics

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Quantum Simulation

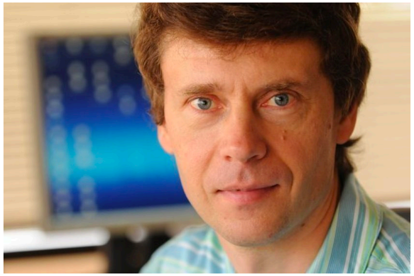
- The goal of quantum simulation is to prepare physical states of interest (ground states or thermal states) and compute physical observables, e.g., n-point correlation functions.
- Quantum computers are powerful, but they do have limitations.
  - Easy: Time-evolution
  - Not-so-easy: Ground state preparation

Potential wish list

- Given a Hamiltonian H, prepare its ground state.
- Given a Hamiltonian H, prepare its thermal state at temperature T.
- Given a Hamiltonian H, apply $\exp(-iHt)$.

Ground state preparation = hard

- Even calculating ground state energy is hard. [Kitaev (1999)]



- In particular, we do not expect the quantum computer to be able to find ground states of classical spin- glass Hamiltonians.

$$\lim_{N\to\infty} \underbrace{(e^{-H\delta t})^N}|0\cdots 0\rangle \propto \underline{|\psi_{g.s.}\rangle}$$

Imaginary time-evolution/thermal state: Not obvious

- Not unitary!
- Possible sometimes [Motta et al., Nature Physics, 16, 205-210 (2020)] but generally not easy.
- Finite-temperature simulation: Possible but convergence generally hard to establish. [Temme et al., Nature, 471, 87-90 (2020)]

Quantum Metropolis algorithm

$H : \{|E_n\rangle\}$

Time evolution: Easy

- In a quantum computer, time evolution can be implemented efficiently.
- This is usually the goal of quantum simulation algorithms.
- There are many approaches
  - Trotter-Suzuki
  - Linear combination of unitaries
  - Qubitization
  - Randomized Trotter-Suzuki,
  - …

Time evolution: Goal

n: # of qubits

- We are given a Hamiltonian H.
- Given $t \in \mathbb{R}$, we want to synthesize a unitary U s.t.

$$\|U - e^{-iHt}\| \leq \epsilon.$$

$\|A\| = \max_{\lambda_i} |\lambda_i|$, λ_i is e.value of A.

- Parameters: ϵ, t, n .
- Key questions
  1. How many gates do we need?
  2. How many qubits do we need?

* Gate set: Clifford + non-Clifford gates ($T = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{i} \end{pmatrix}$, Toffoli)

Trotter-Suzuki method

- Basic idea: $e^{A_1+A_2+\ldots A_n} = \lim_{m\to\infty} \left(\underbrace{e^{A_1/m}e^{A_2/m}\ldots e^{A_n/m}}\right)^m$.

$\lim_{m\to\infty} e^{\frac{A_1}{m}} \approx I + \frac{A_1}{m}$

e^{-itH}

$H = \sum_{i=1}^{N} h_i$

Trotter-Suzuki method

- Consider the following toy model.

$$H = -t\sum_i (\underbrace{a_i^\dagger}_{\text{creation}}\underbrace{a_{i+1}}_{\text{annihilation}} + h.c.) + U\sum_i \hat{n}_i\hat{n}_{i+1}. \qquad (\{a_i^\dagger, a_j\} = \delta_{ij})$$

$e^{-i\Delta H}$

Δ: Time

Trotter-Suzuki method

$e^{-\beta H}$ $\quad e^{-\beta X_1 X_2}$ $\quad e^{-itH}$ $\quad e^{-\beta H}$

$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

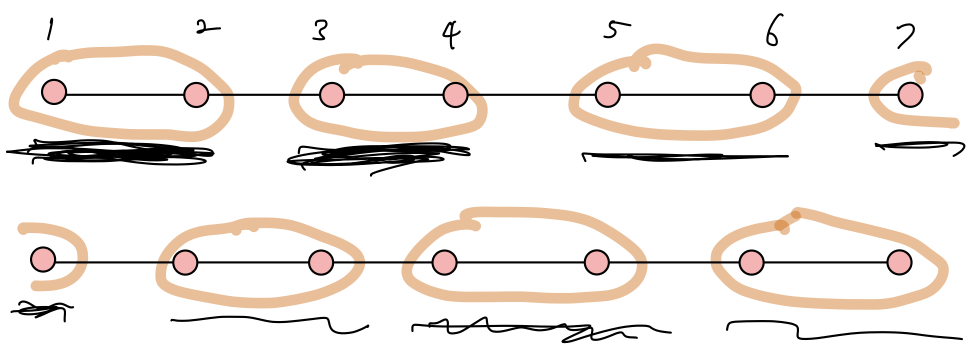
$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

- Jordan-Wigner transformation

$$H = -\frac{t}{2}\sum_i (X_iX_{i+1} + Y_iY_{i+1}) + U\sum_i \frac{(Z_i+1)(Z_{i+1}+1)}{4}.$$

Even



$H_{even} = h_{12} + h_{34} + h_{56} + \cdots$

$H_{odd} = h_1 + h_{23} + h_{34} + \cdots$

Odd

$H = H_{even} + H_{odd}$

$$e^{-iH\Delta} = e^{-i(H_{even}+H_{odd})\Delta} \underset{\Delta\simeq 0}{\approx} e^{-i(H_{even})\Delta}\, e^{-iH_{odd}\Delta}$$

Trotter-Suzuki method

1. Break down to 3x2= 6 layers.
2. Each layer can be implemented straightforwardly.

$$e^{i(X_1X_2)\Delta t/2}$$
$$e^{i(Y_1Y_2)\Delta t/2}$$
$$e^{-i\frac{U}{4}(Z_1+1)(Z_2+1)}$$

$$H = -\frac{t}{2}\sum_i (X_iX_{i+1} + Y_iY_{i+1}) + U\sum_i \frac{(Z_i+1)(Z_{i+1}+1)}{4}.$$

- Q: Complexity of a single Trotter step?

$e^{i(X_1X_2)\Delta t/2}$ Clifford: 2

non-Clifford: $3\log_2(1/\epsilon)+\dots$ (T)

$e^{iX_1X_2\theta}$

$e^{iX_1X_2\theta} = CNOT_{1,2}\, e^{iX_1\theta}\, CNOT_{1,2}$

$* \; CNOT_{1,2}\, X_1\, CNOT_{1,2} \overset{?}{=} X_1X_2$

$* \; CNOT_{1,2}\, |0\rangle_1|0\rangle_2 = |0\rangle|0\rangle$

$|0\rangle_1|1\rangle_2 = |0\rangle|1\rangle$

$|1\rangle_1|0\rangle_2 = |1\rangle|1\rangle$

$|1\rangle_1|1\rangle_2 = |1\rangle|0\rangle$

$\xrightarrow{X_1}$ $|1\rangle|0\rangle$, $|1\rangle|1\rangle$, $|0\rangle|1\rangle$, $|0\rangle|0\rangle$ $\xrightarrow{CNOT_{1,2}}$ $|1\rangle|1\rangle$, $|1\rangle|0\rangle$, $|0\rangle|1\rangle$, $|0\rangle|0\rangle$

$CNOT^2 = I$

Total T-gate cost $= O(n \log_2(1/\varepsilon))$
(for a single Trotter step)

Trotter-Suzuki method

- Now consider a different toy model, now in 2D.

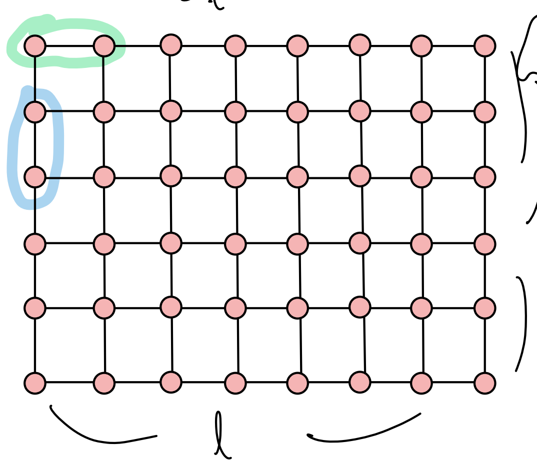
$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + h.c.) + U \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j .$$

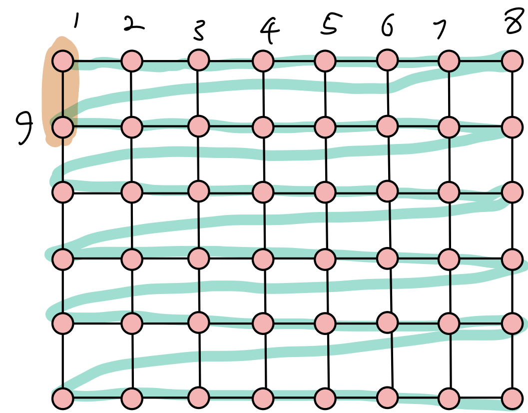
$\frac{1+Z_i}{2} \frac{1+Z_j}{2}$

$a_i^\dagger a_j + h.c.$ $\begin{cases} x: \frac{X_i X_j + Y_i Y_j}{2} \\ y: \frac{X_1 Z_2 \cdots Z_8 X_9 + Y_1 Z_2 \cdots Z_8 Y_9}{2} \end{cases}$

$2\ell^2$ $2\ell^2$

$\boxed{2(|t| + |U|)\,\ell^2}$





Trotter-Suzuki method

1. Apply Jordan-Wigner transformation.
2. Break down to 3 x 2^2 = 12 layers.
3. Now we need to deal with non-local gates.

$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + h.c.) + U \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j .$$

CNOTS $X_1 Z_1 \cdots Z_n X_{n+1}$ CNOTS $= X_1 Z_n X_{n+1}$

$$e^{i\theta \frac{1}{2}(XZ \cdots ZX + YZ \cdots ZY)}$$

* Identity: $CNOT_{2,1} Z_1 CNOT_{2,1} = Z_1 Z_2$

$|0\rangle|0\rangle$, $|0\rangle|1\rangle$, $|1\rangle|0\rangle$, $|1\rangle|1\rangle$ $\xrightarrow{CNOT_{2,1}}$ $|0\rangle|0\rangle$, $|1\rangle|1\rangle$, $|1\rangle|0\rangle$, $|0\rangle|1\rangle$ $\xrightarrow{Z_1}$ $|0\rangle|0\rangle$, $-|1\rangle|1\rangle$, $-|1\rangle|0\rangle$, $|0\rangle|1\rangle$ $\xrightarrow{CNOT_{2,1}}$ $|0\rangle|0\rangle$, $-|0\rangle|1\rangle$, $-|1\rangle|0\rangle$, $|1\rangle|1\rangle$ $=$ $Z_1Z_2|0\rangle|0\rangle$, $Z_1Z_2|0\rangle|1\rangle$, $Z_1Z_2|1\rangle|0\rangle$, $Z_1Z_2|1\rangle|1\rangle$

[illegible] $n + O(1)$

Clifford : 2 n (...)

non-Clifford: $3 \log_2(1/\epsilon) + \cdots$

Non-local gates

- Non-local gates here are of the following form.

  $e^{i\theta(XZ\ldots ZX+YZ\ldots ZY)}$

  How many gates do we need to implement this?

Trotter-Suzuki: Pros and Cons

- Pros
  - ❖ Conceptually simple
  - ❖ Efficient, formally speaking
  - ❖ Works well in practice
- Cons
  - ❖ Far from optimal (compared to other methods)

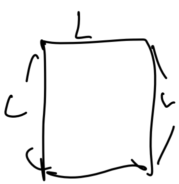
ε, t, n

Trotter-Suzuki method

- Trotter-Suzuki method is efficient and works reasonably well for toy models.
- However, for realistic Hamiltonians (appearing in quantum chemistry), Trotter-Suzuki is not the leading approach, at least for now.
- However, there have been some interesting developments. Trotter-Suzuki method may work very well in practice.

Trotter-Suzuki method: Recent developments

- Randomization method: "A random compiler for fast Hamiltonian simulation", Campbell (2018).
- Better bound: "A Theory of Trotter Error," Childs *et al.* (2019).
- Works better at low energies: "Hamiltonian simulation in the low energy subspace," Sahinoglu and Somma (2021). (Theoretical)



1D: $O(L)$

2D: $O(L^2 \times L)$ non-locality

3D: $O(L^3 \times L^2)$

$O(L^2)$

$O(L^3)$

Summary

- State preparation: Generally hard.
- Time evolution: Easy
- Trotter-Suzuki: The simplest Hamiltonian Simulation method. Works pretty well in practice!