6. Hamiltonian Simulation (LCU): pt.2

Isaac H. Kim (UC Davis)

SELECT & PREPARE Costs

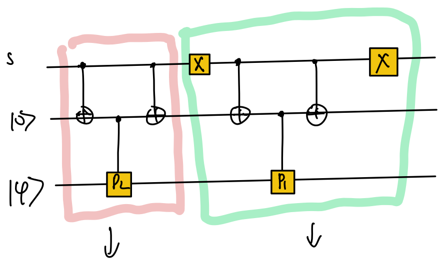
$\{P_1, P_2\}$

$|0\rangle_s|\psi\rangle \rightarrow |0\rangle_s P_1|\psi\rangle$

$|1\rangle_s|\psi\rangle \rightarrow |1\rangle_s P_2|\psi\rangle$

0 : → Nothing → P_1

1 : → P_2 → P_2



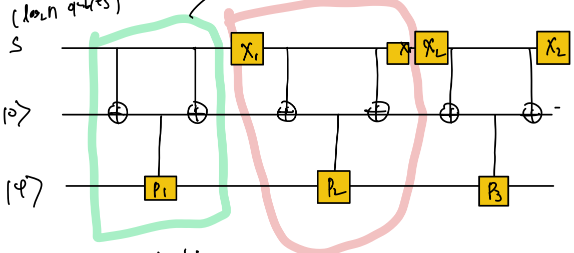
P_2 only if $s=1$

P_1 only if $s=0$

$\{P_1, P_2, \dots P_n\}$

n stages

(log n qubits)



P_1 only if $s=0\dots0$

P_2 only if $s=0\dots01$

n Paulis → $O(n \log n)$

$O(n)$

Summary

- In the Trotter-based Hamiltonian simulation, there is an inevitable $O(poly(\epsilon^{-1}))$ scaling in the precision ϵ .
- Using the LCU approach, one can get a sub-logarithmic scaling in $1/\epsilon$. [Berry, Childs, Cleve, Kohtari, and Somma (2013, 2014)]
- Using SELECT + PREPARE, we can apply the desired unitary with a nonzero probability.
- However, we haven't discussed how to boost this probability. We'll talk about that in this lecture.

Amplitude amplification

- One potential issue here is that the success probability is low. If we apply the same operation many times, with high probability we will fail.
- Fortunately, there is a well-known way to amplify the amplitude, aka amplitude amplification. [Brassard, Hoyer, Mosca, and Tapp (2000)]

Basic Setup

- $|0\rangle = \overset{\sin}{\cancel{\cos}}(\theta)\,|\psi\rangle + \overset{\cos}{\cancel{\sin}}(\theta)\,|\psi_\perp\rangle$.
- $R_0 = I - 2\,|0\rangle\langle 0|$ $= I - 2|0\rangle(\langle\psi|\cos\theta + \langle\psi_\perp|\sin\theta)$
- $R_\psi = I - 2\,|\psi\rangle\langle\psi|$
- $R_0R_\psi(\underset{\sin}{\cancel{\cos}}(\theta)\,|\psi\rangle + \underset{\cos}{\cancel{\sin}}(\theta)\,|\psi_\perp\rangle) = ?$

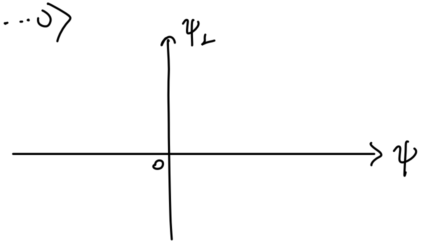
Incorrect

$\cancel{\boxed{\overset{\sin}{\cancel{\cos}}(2\theta)|\psi\rangle + \overset{\cos}{\cancel{\sin}}(2\theta)|\psi_\perp\rangle}}$

$\sin((2t+1)\theta)|\psi\rangle + \cos((2t+1)\theta)|\psi_\perp\rangle$

$|\psi\rangle,\ |\psi_\perp\rangle$

$|0\rangle = |0\cdots0\rangle$



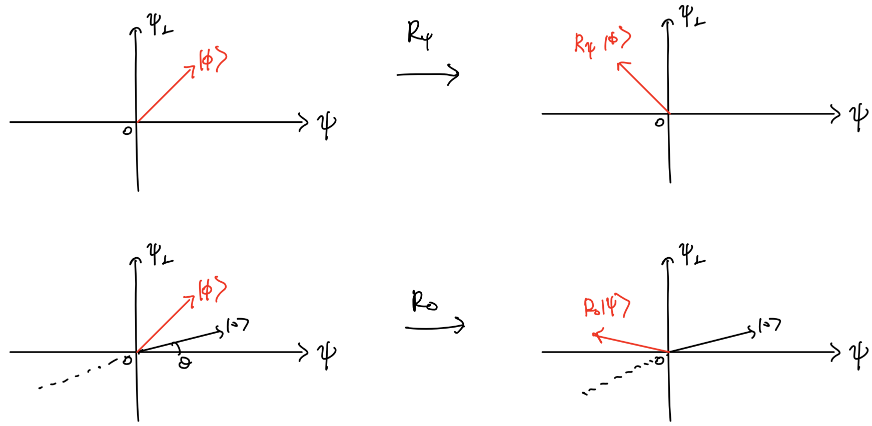
$R_\psi|\psi\rangle = -|\psi\rangle$

$R_\psi|\psi_\perp\rangle = |\psi_\perp\rangle$

$R_0|\psi\rangle \overset{?}{=} |\psi\rangle - 2|0\rangle(\langle\psi|\cos\theta + \langle\psi_\perp|\sin\theta)|\psi\rangle$

$= |\psi\rangle - 2\cos\theta|0\rangle$

$R_0|\psi_\perp\rangle$



ψ⊥
|ϕ⟩
ψ
0
Rψ
Rψ|ϕ⟩
|ϕ⟩
|0⟩
θ
R0
R0|ψ⟩

Quiz

- Can we prepare $|\psi\rangle$ exactly?

If $\theta = \frac{\pi}{2(2n+1)}$ for an integer n, the answer is obviously yes. But what about general θ?

$$|0\cdots 0\rangle = \sin\theta|\psi\rangle + \cos\theta|\psi_\perp\rangle$$

$$R_0 = I - 2|0\cdots 0\rangle\langle 0\cdots 0|$$

$$R_\psi = I - 2|\psi\rangle\langle\psi|$$

$$|0\cdots 0\rangle|0\rangle = \sin\theta'|\tilde{\psi}\rangle + \cos\theta'|\tilde{\psi}_\perp\rangle$$

$$\tilde{R}_0 = I - 2(|0\cdots 0\rangle\langle 0\cdots 0| \otimes |0\rangle\langle 0|)$$

$$\tilde{R}_\psi = I - 2|\psi\rangle\langle\psi| \otimes |\phi\rangle\langle\phi|$$

$$|\tilde{\psi}\rangle = |\psi\rangle \otimes |\phi\rangle$$

$$\sin\theta' = \sin\theta \, \langle 0|\phi\rangle$$

Given θ, find the smallest n s.t. $\frac{\pi}{2n} \leq \theta$

$$\sin\frac{\pi}{2n} = \sin\theta \, \langle 0|\phi\rangle$$

Oblivious Amplitude amplification

- Unfortunately, amplitude amplification is not exactly what we want.
- In amplitude amplification, ~~if~~ we can prepare a specific *state* we want. But what we actually want is to apply a specific *unitary* to an arbitrary state.

Oblivious Amplitude amplification: Setup

- $U|\psi\rangle_A|0\rangle_B = \overset{\sin\theta}{\cancel{\cos(\theta)}} V|\psi\rangle_A|0\rangle_B + \overset{\cos\theta}{\cancel{\sin(\theta)}}|\phi\rangle_A|1\rangle_B$.
- $R_0 = I - 2|0\rangle_B\langle 0|$
- Goal: Implement $|\psi\rangle_A|0\rangle_B \to V|\psi\rangle_A|0\rangle_B$

$e^{-iHt} \cong \sum \alpha_p P$ — SELECT, PREPARE

$\langle 0\cdots 0|$ PREPARE† SELECT PREPARE $(|\psi\rangle|0\cdots 0\rangle) = \sum_p \alpha_p P|\psi\rangle$

$\updownarrow$

PREPARE† SELECT PREPARE $(|\psi\rangle|0\cdots 0\rangle) = \left(\sum_p \alpha_p P|\psi\rangle|0\cdots 0\rangle\right) + |\text{Junk}\rangle$

$(\langle 0\cdots 0|\otimes I)|\text{Junk}\rangle = 0$

Oblivious Amplitude Amplification

Let $S = -URU^\dagger R$, where $R = 2|0\rangle\langle 0| - I$. Then we have

$$S^\ell U|0\rangle|\psi\rangle = \sin((2\ell+1)\theta)|0\rangle V|\psi\rangle + \cos((2\ell+1)\theta)|1\rangle|\phi\rangle.$$

[Berry, Childs, Cleve, Kothari, and Somma (2014)]

$(2l+1)\theta = \frac{\pi}{2}$

$\Downarrow$

$S^l U|0\rangle|\psi\rangle = |0\rangle V|\psi\rangle$

$H = \sum_i Z_i Z_{i+1}$

e^{-itH}

$\mathrm{SELECT}\,|i\rangle|\psi\rangle = |i\rangle Z_i Z_{i+1}|\psi\rangle$

$\mathrm{PREPARE}|0\cdots0\rangle = \sum_{i=1}^{n} \frac{1}{\sqrt{n}}|i\rangle$

LCU: Putting everything together

n : # of qubits
T : sim time
ε : Error

- Gate cost analysis
  - Simulation time: (Almost) linear
  - Precision: (Almost) logarithmic
- To get a reasonable gate cost estimate, one can simply multiply the cost of implementing SELECT/PREPARE subroutines.

Cost of SELECT

- Naive approach: $O(N \log N)$
- A smarter approach: $O(N)$
- State-of-the-art: Low, Kliuchnikov, Schaeffer (2018)
  - Sub-linear scaling in N possible (for T-gates), provided that you're willing to use more qubits.
  - Optimal

Cost of PREPARE

- Naive approach: $O(N \log(N/\epsilon))$ [Shende, Bullock, and Markov (2006)]
- Better data structure: $O(N + \log(1/\epsilon))$ [Babbush et al. (2018)]
- State-of-the-art: Low, Kliuchnikov, Schaeffer (2018)
  - Sub-linear scaling in N possible (for T-gates), provided that you're willing to use more qubits.

Playing with non-unitary operators

- It is possible to apply a linear combination of unitary, even if it results in a non-unitary operator. (LCU)
- Even if you can apply a unitary operator probabilistically, you can boost the success probability to 1, making the operation deterministic. (Oblivious amplitude amplification)
- A natural question: Can we apply a *non-unitary operator* and boost the success probability?

e^{-iHt} → Taylor expansion [SELECT / PREPARE