Quantum Algorithms for Hamiltonian Simulation

M. Sohaib Alam

NASA QuAIL / USRA, Ames Research Center

SQMS/GGI Summer School, July 2022

General Idea

Goal: For a given Hamiltonian *H*, find a (compilable) unitary *U* such that for any $\epsilon > 0$ and t > 0

$$||U - e^{-iHt}|| < \epsilon$$

Allows us to simulate the time dynamics

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

May require ancillary qubits

$$||U|\bar{0}\rangle|\psi\rangle - |\bar{0}\rangle e^{-iHt}|\psi\rangle|| < \epsilon$$

Simulation Methods

- Lie-Trotter-Suzuki
- Linear Combination of Unitaries (LCU)
- Qubitization

Encodings

Fermions

$$\{a_p, a_q^\dagger\} = \delta_{pq}$$

$$\{a_p, a_q\} = \{a_p^\dagger, a_q^\dagger\} = 0$$

(Jordan-Wigner) $\Rightarrow$

$$a_p = \frac{1}{2}(X + iY) \otimes Z_{p-1} \otimes \cdots \otimes Z_0$$

$$a_p^\dagger = \frac{1}{2}(X - iY) \otimes Z_{p-1} \otimes \cdots \otimes Z_0$$

Bosons

$$[a_p, a_q^\dagger] = \delta_{pq}$$

$$[a_p, a_q] = [a_p^\dagger, a_q^\dagger] = 0$$

(Truncated occupation number) $\Rightarrow$

$$a^\dagger = \begin{pmatrix} 0 & 0 & 0 & \dots \\ 1 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & \dots \\ \vdots & & \ddots & \end{pmatrix}$$

Suzuki-Lie-Trotter

N-qubit *k*-local Hamiltonian

$$H = \sum_i H_i \qquad [H_i, H_j] \neq 0$$

Baker-Campbell-Hausdorff (BCH)

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A,[A,B]]+\ldots}$$

Suzuki-Lie-Trotter

Lie-Trotter product formula

$$e^{-iHt} = \lim_{n\to\infty} \left(e^{-iH_1 t/n} e^{-iH_2 t/n} \ldots e^{-iH_m t/n} \right)^n$$

Algorithm:

- Exponentiate each of the k-local terms in succession
- Repeat a large number of times

Suzuki-Lie-Trotter

$$e^{-iHt} \approx \left(e^{-iH_1 t/n} e^{-iH_2 t/n} \ldots e^{-iH_m t/n}\right)^n + O\left(\frac{t^2}{n}\right)$$

C_H : (Max) Cost of implementing any single $e^{-iH_i t/n}$ term

m: Total number of k-local terms

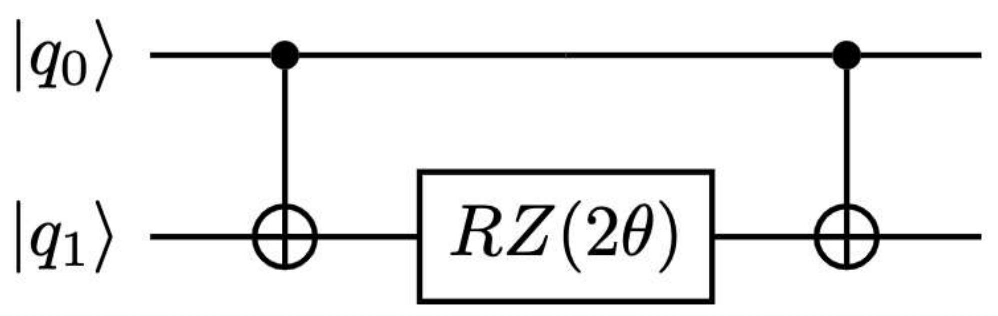
ϵ : Desired accuracy

$$\text{Total cost } \sim O\left(\frac{mt^2 C_H}{\epsilon}\right)$$

Suzuki-Lie-Trotter

$$
ZZ: \begin{array}{rcl} |00\rangle & \rightarrow & +|00\rangle \\ |01\rangle & \rightarrow & -|01\rangle \\ |10\rangle & \rightarrow & -|10\rangle \\ |11\rangle & \rightarrow & +|11\rangle \end{array} \quad \Rightarrow \quad e^{-i\theta ZZ}: \begin{array}{rcl} |00\rangle & \rightarrow & e^{-i\theta}|00\rangle \\ |01\rangle & \rightarrow & e^{+i\theta}|01\rangle \\ |10\rangle & \rightarrow & e^{+i\theta}|10\rangle \\ |11\rangle & \rightarrow & e^{-i\theta}|11\rangle \end{array}
$$

$$
RZ(\theta) = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix}
$$



Suzuki-Lie-Trotter

Pauli Z's produce XOR in phases

$$Z_i Z_j |b_i\rangle|b_j\rangle = (-1)^{b_i \oplus b_j} |b_i\rangle|b_j\rangle$$

More generally,

$$Z_1 \dots Z_k |b_1\rangle \dots |b_k\rangle = (-1)^{b_1 \oplus \cdots \oplus b_k} |b_1\rangle \dots |b_k\rangle$$

So that

$$e^{-i\theta Z_1 \dots Z_k} |b_1 \dots b_k\rangle = RZ(2\theta)|b_1 \oplus \cdots \oplus b_k\rangle$$

XOR

b_i	b_j	$b_i \oplus b_j$
0	0	0
0	1	1
1	0	1
1	1	0

$$b_i \oplus b_i = 0$$

Controlled NOT (bitflip) produces XOR on bits

$$\mathrm{C}_i\text{-NOT}_j |b_i\rangle|b_j\rangle = |b_i\rangle|b_i \oplus b_j\rangle$$

$$\mathrm{C}_i\text{-NOT}_j |b_i\rangle|b_i \oplus b_j\rangle = |b_i\rangle|b_i \oplus b_i \oplus b_j\rangle = |b_i\rangle|b_j\rangle$$

Suzuki-Lie-Trotter

Prescription to compile $e^{-i\theta Z_1 \ldots Z_k}$

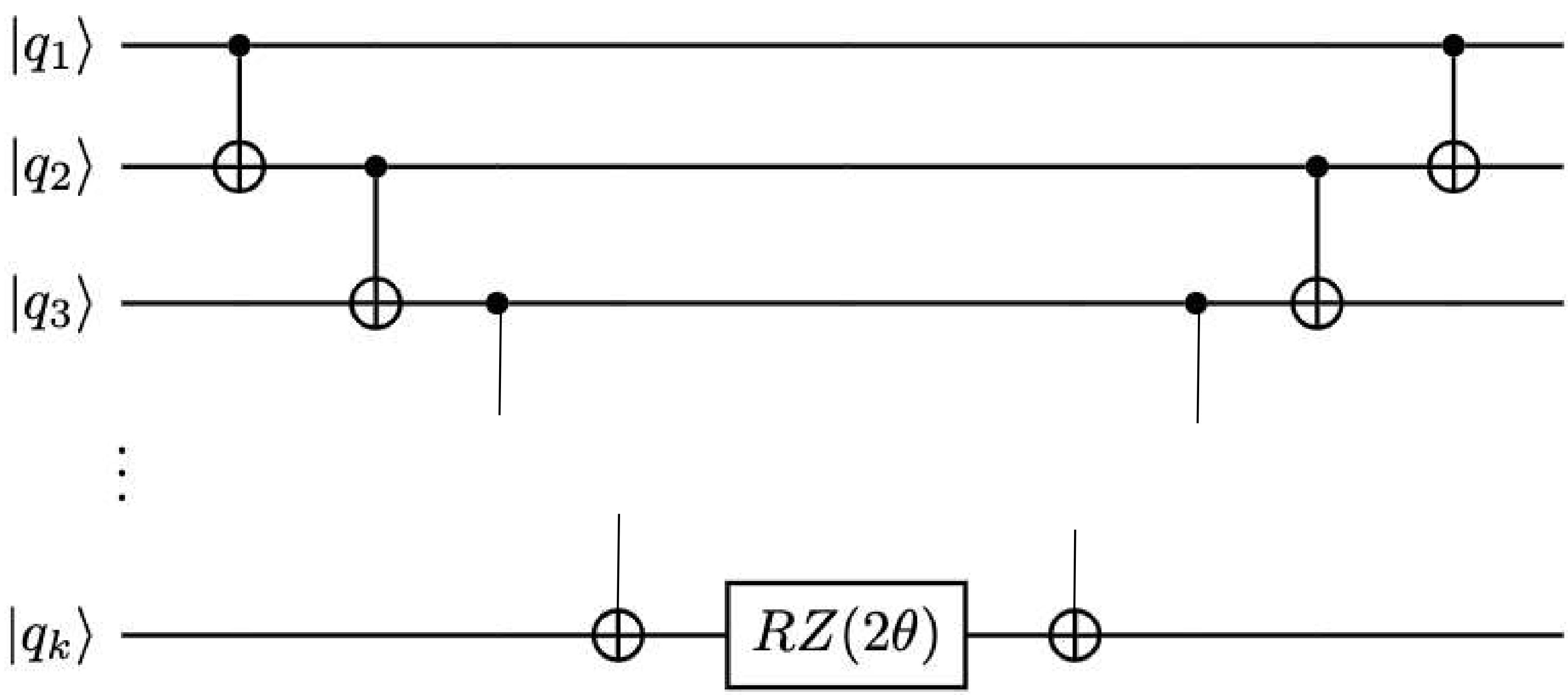
- $$\prod_{i=1}^{k-1} \mathrm{C}_i\text{-}\mathrm{NOT}_{i+1} |b_1\rangle \ldots |b_k\rangle = |b_1\rangle |b_1 \oplus b_2\rangle \ldots |b_1 \oplus b_2 \oplus \cdots \oplus b_k\rangle$$

- $$RZ_k(2\theta)|b_1\rangle \ldots |b_1 \oplus b_2 \oplus \cdots \oplus b_k\rangle = e^{-i\theta(-1)^{b_1 \oplus \cdots \oplus b_k}} |b_1\rangle \ldots |b_1 \oplus b_2 \oplus \cdots \oplus b_k\rangle$$

- $$\prod_{i=k-1}^{1} \mathrm{C}_{i-1}\text{-}\mathrm{NOT}_i |b_1\rangle |b_1 \oplus b_2\rangle \ldots |b_1 \oplus b_2 \oplus \cdots \oplus b_k\rangle = |b_1\rangle \ldots |b_k\rangle$$

Suzuki-Lie-Trotter

$$e^{-i\theta Z_1 \ldots Z_k}$$



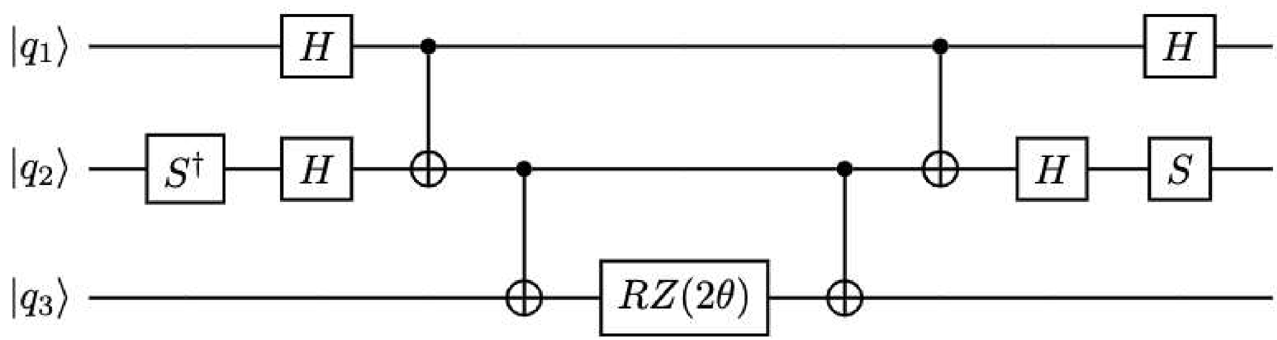
Suzuki-Lie-Trotter

Note that

$$X = HZH \qquad\qquad Y = (SH)Z(SH)^\dagger$$

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

E.g. $e^{-i\theta X_1 Y_2 Z_3}$



Suzuki-Lie-Trotter

$$e^{-iHt} \approx \left(e^{-iH_1 t/n} e^{-iH_2 t/n} \dots e^{-iH_m t/n}\right)^n + O\left(\frac{t^2}{n}\right)$$

C_H : (Max) Cost of implementing any single $e^{-iH_i t/n}$ term

m: Total number of k-local terms

ϵ : Desired accuracy

$$\text{Total cost } \sim O\left(\frac{mt^2 C_H}{\epsilon}\right) \sim O\left(\frac{mt^2 k}{\epsilon}\right)$$

Suzuki-Lie-Trotter

Suzuki higher-order formulas

$$S_2(\Delta t) = e^{-iH_1\Delta t/2} \dots e^{-iH_{m-1}\Delta t/2} e^{-iH_m\Delta t} e^{-iH_{m-1}\Delta t/2} \dots e^{-iH_1\Delta t/2}$$

yields a better approximation

$$e^{-iH\Delta t} = S_2(\Delta t) + O(\Delta t^3)$$

Recursive definition

$$S_{2k}(\Delta t) = \left[S_{2(k-1)}(p_k\Delta t)\right]^2 S_{2(k-1)}(q_k\Delta t) \left[S_{2(k-1)}(p_k\Delta t)\right]^2$$

$$p_k = \left(4 - 4^{1/(2k-1)}\right)^{-1}, \quad q_k = 1 - 4p_k$$

$$e^{-iH\Delta t} = S_{2k}(\Delta t) + O(\Delta t^{2k+1})$$

Linear Combination of Unitaries

Taylor series expansion

$$e^{-iHt} = \left(\underbrace{e^{-iH(t/r)}}\right)^r$$

$$V_r = \sum_{k=0}^{\infty} \frac{1}{k!}\left(\frac{-iHt}{r}\right)^k$$

$$\approx \sum_{k=0}^{K} \frac{1}{k!}\left(\frac{-iHt}{r}\right)^k$$

Implement $\tilde{V} = \sum_i \alpha_i U_i$ such that $||\tilde{V} - V_r|| < \epsilon/r$

Linear Combination of Unitaries

Given

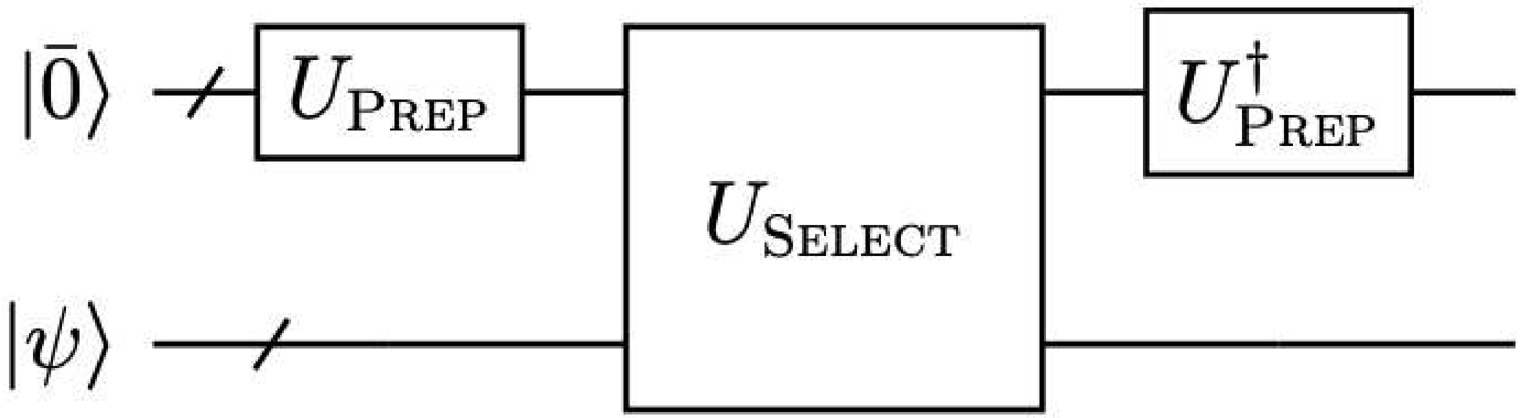
$$H = \sum_{i=1}^{L} \alpha_i U_i \qquad \alpha_i > 0$$

Construct

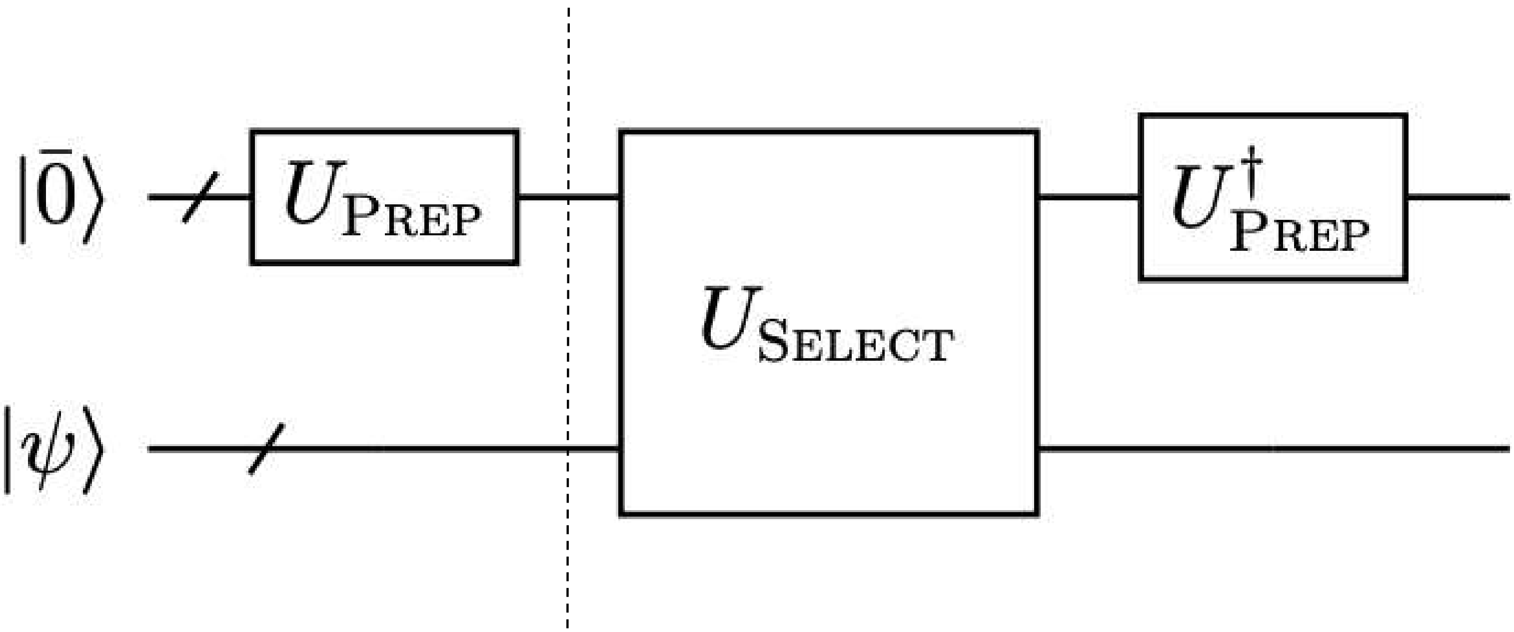
$$U_{PREP}|\bar{0}\rangle = \frac{1}{\sqrt{|\alpha|_1}} \sum_{i=1}^{L} \sqrt{\alpha_i}|i\rangle \qquad |\alpha|_1 = \sum_{i=1}^{L} \alpha_i$$

$$U_{SELECT} = \sum_{i=1}^{L} |i\rangle\langle i| \otimes U_i$$

Linear Combination of Unitaries

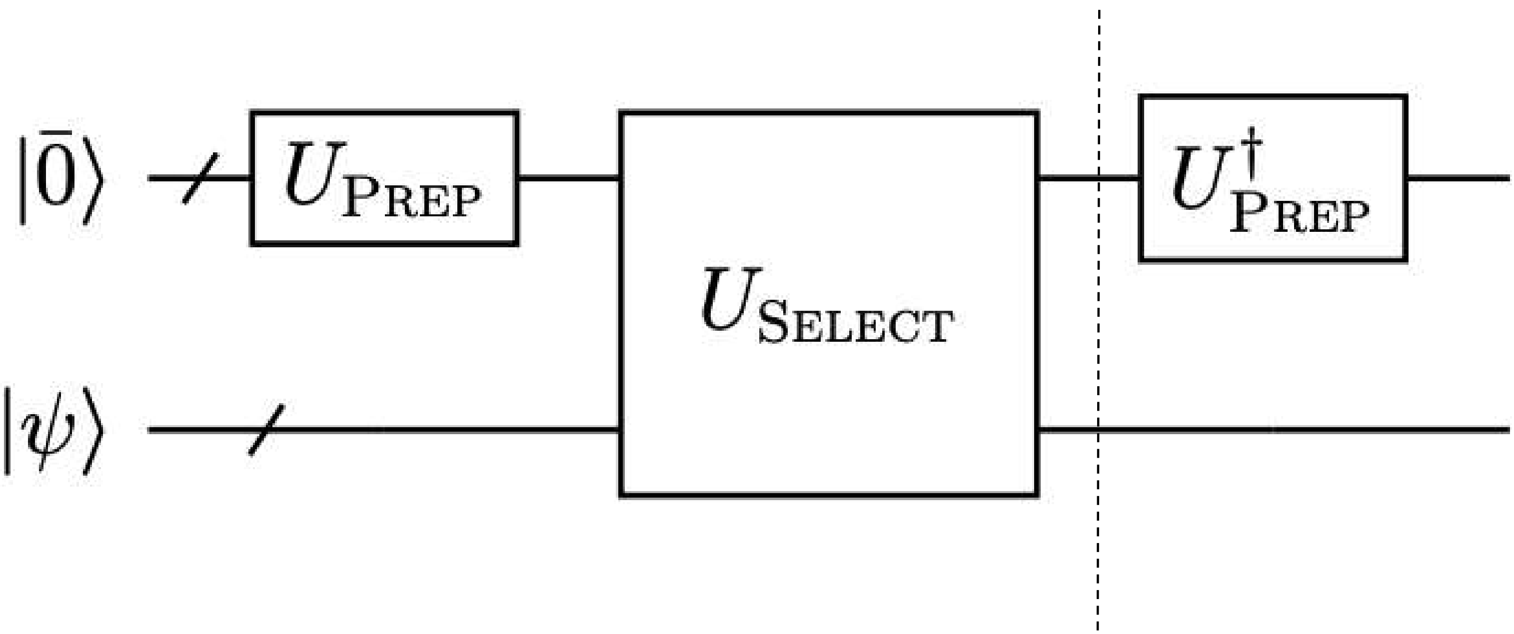


Linear Combination of Unitaries



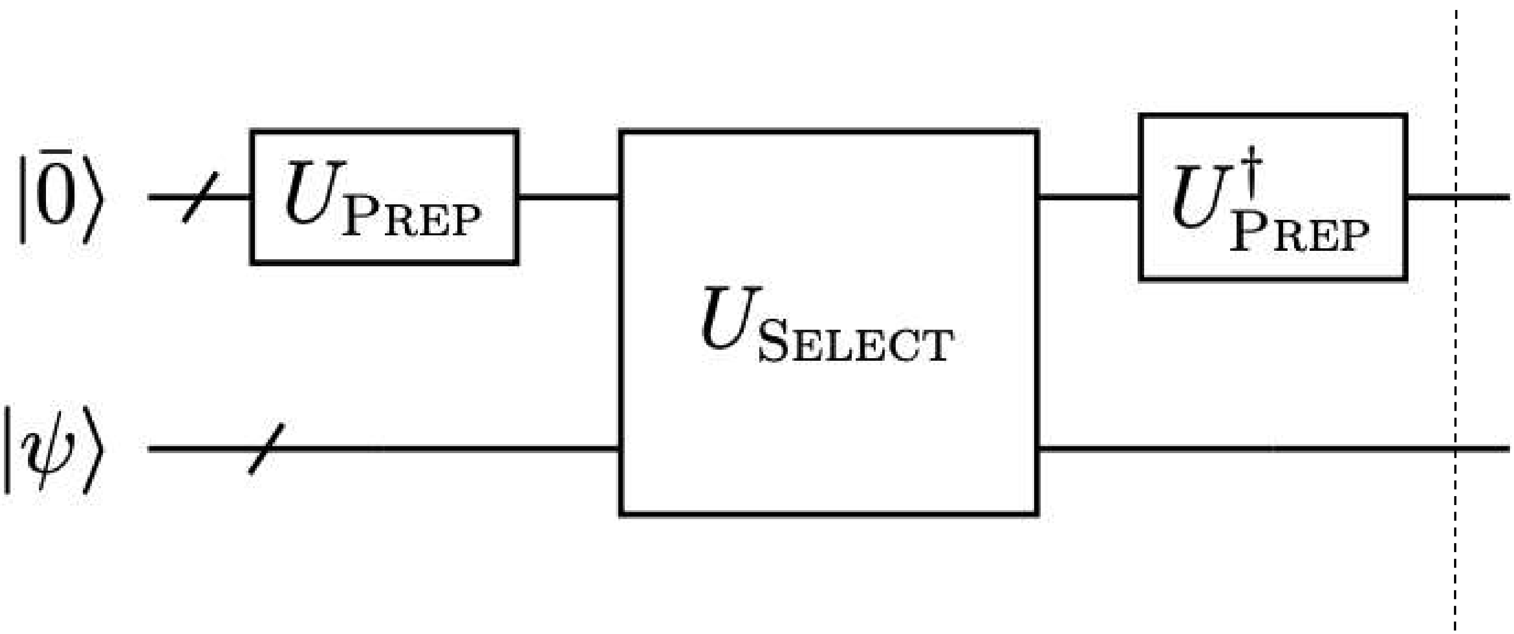
$$\left(\frac{1}{\sqrt{|\alpha|_1}}\sum_{i=1}^{L}\sqrt{\alpha_i}|i\rangle\right)\otimes|\psi\rangle$$

Linear Combination of Unitaries



$$\frac{1}{\sqrt{|\alpha|_1}} \sum_{i=1}^{L} \sqrt{\alpha_i}|i\rangle \otimes U_i|\psi\rangle$$

Linear Combination of Unitaries



Success probability

$$\frac{||A|\psi\rangle||^2}{||\alpha||_1^2}$$

$$\frac{1}{|\alpha|_1}|\bar{0}\rangle \otimes A|\psi\rangle + |\Phi^{\perp}\rangle$$

$$\left(|\bar{0}\rangle\langle\bar{0}| \otimes \mathbb{I}\right)|\Phi^{\perp}\rangle = 0$$

Linear Combination of Unitaries

Robust Oblivious Amplitude Amplification

Let $W|\bar{0}\rangle|\psi\rangle = \frac{1}{s}|\bar{0}\rangle\tilde{V}|\psi\rangle + \sqrt{1-\frac{1}{s^2}}|\Phi^{\perp}\rangle$

If $||s-2|| \sim O(\epsilon),\ \text{and}\ ||\tilde{V}-V|| \sim O(\epsilon)$ where V is unitary, then with the reflection operator $R = 2\left(|\bar{0}\rangle\langle\bar{0}| \otimes \mathbb{I}_s\right) - \mathbb{I}$,

the unitary $A = WRW^{\dagger}RW$ achieves

$$||A|\bar{0}\rangle|\psi\rangle - |\bar{0}\rangle V|\psi\rangle|| \sim O(\epsilon)$$

Qubitization

Suppose $H = \langle g|U|g\rangle$

Then $W_U = (2|\tilde{g}\rangle\langle\tilde{g}| \otimes \mathbb{I}_s - \mathbb{I})\tilde{U}$ defines a step of a "quantum walk"

$$\tilde{U} = |0\rangle\langle 1|_c \otimes U + |1\rangle\langle 0|_c \otimes U^\dagger$$

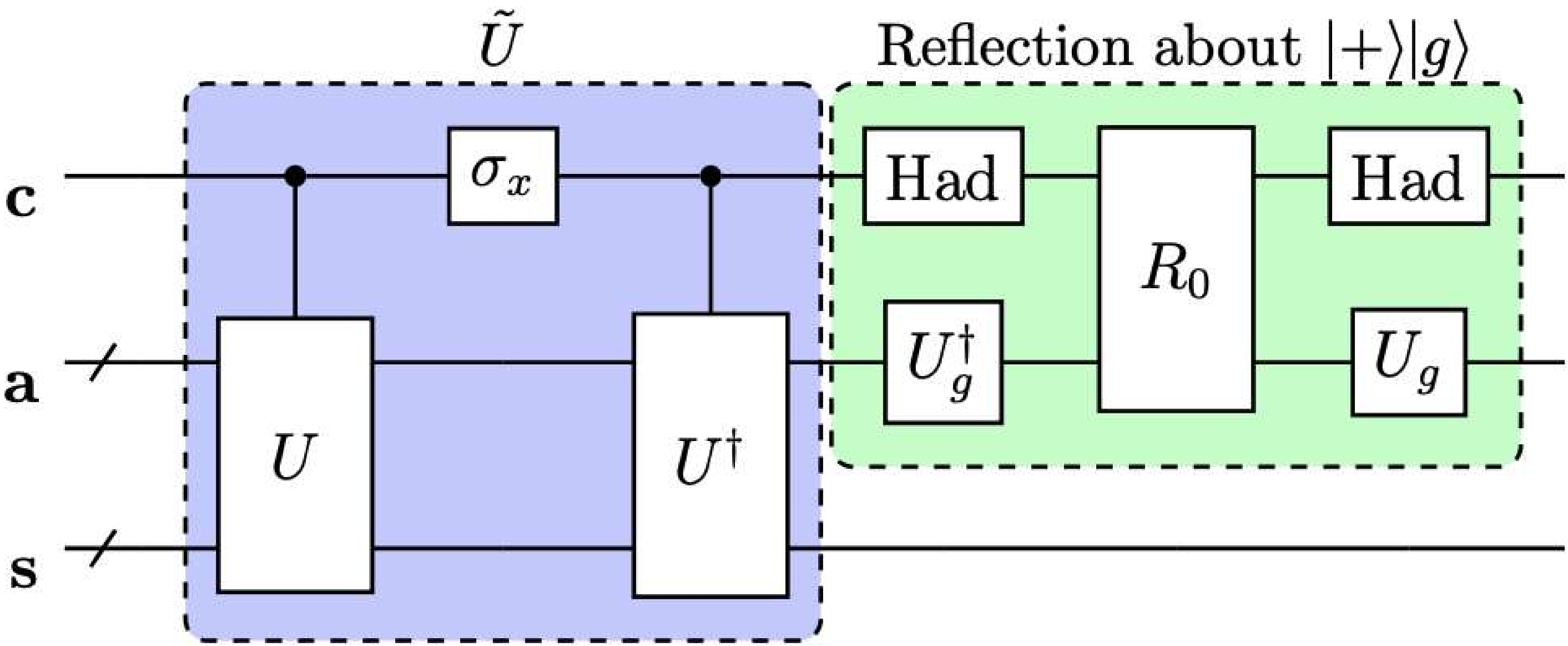
$$|\tilde{g}\rangle = |+\rangle_c|g\rangle$$

Qubitization

We can construct $H = \langle g|U|g\rangle$

using $|g\rangle = U_{PREP}|\bar{0}\rangle$ $U = U_{SELECT}$

Qubitization



Qubitization

Jacobi-Anger

$$S_K = \sum_{k=-K}^{K} a_k \left(-iW_U\right)^k$$

$$W_U = \oplus_j \begin{pmatrix} \lambda_j & -\sqrt{1-\lambda_j^2} \\ \sqrt{1-\lambda_j^2} & \lambda_j \end{pmatrix}$$

Thank you!

Email: sohaib.alam@nasa.gov;
malam@usra.edu