Quantum Algorithms for Hamiltonian Simulation

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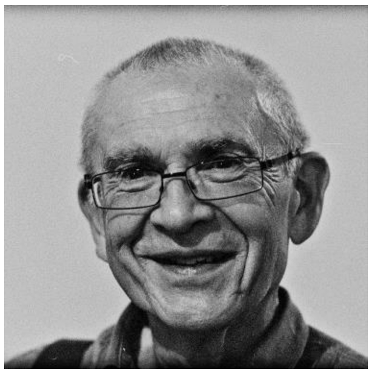
NASA QuAIL / USRA, Ames Research Center

SQMS/GGI Summer School, July 2022

General Idea



Yuri Manin, *"Computable and Uncomputable"* (1980)

Richard Feynman, *"Simulating physics with computers"* (1982)

> phenomena—the challenge of explaining quantum mechanical phenomena —has to be put into the argument, and therefore these phenomena have to be understood very well in analyzing the situation. And I'm not happy with all the analyses that go with just the classical theory, because 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. Thank you.

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

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

Simulation Methods

- Lie-Trotter-Suzuki (Trotterization)
- Linear Combination of Unitaries (LCU)
- Quantum Singular Value Transform (QSVT)

Encodings

$$H_{system} \rightarrow \sum_i \alpha_i P_i \qquad\qquad |\psi\rangle_{system} \rightarrow \sum_j \beta_j |j\rangle$$

(Jordan-Wigner)

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

$$\Rightarrow$$

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

("Second quantization")

$$\psi(\mathbf{x_0} \ldots \mathbf{x_{N-1}}) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_0(\mathbf{x_0}) & \phi_1(\mathbf{x_0}) & \ldots & \phi_{M-1}(\mathbf{x_0}) \\ \phi_0(\mathbf{x_1}) & \phi_1(\mathbf{x_1}) & \ldots & \phi_{M-1}(\mathbf{x_1}) \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \phi_0(\mathbf{x_{N-1}}) & \phi_1(\mathbf{x_{N-1}}) & \ldots & \phi_{M-1}(\mathbf{x_{N-1}}) \end{vmatrix} = |f_{M-1}, \ldots, f_p, \ldots, f_0\rangle$$

(Field-amplitude basis)

$$\hat{\phi} = \begin{pmatrix} -\phi_{max} & \cdots & \\ & -\phi_{max} + \Delta\phi & \\ \vdots & \ddots & \\ & & \phi_{max} \end{pmatrix}$$

Suzuki-Lie-Trotter

N-qubit *k*-local Hamiltonian

$$H = \sum_{i=1}^{m} H_i$$

$$[H_i, H_j] \neq 0$$

E.g. 5-qubit 2-local

$$H = X_1 Y_3 + Z_2 Z_5 + X_3 Y_4 + Z_1 X_5$$

Baker-Campbell-Hausdorff (BCH)

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

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

$$e^{-iHt} = \left(e^{-iH\Delta t}\right)^n \qquad \Delta t = t/n$$

$$e^{-iH\Delta t} \approx e^{-iH_1\Delta t} \ldots e^{-iH_m\Delta t} + O(\Delta t^2)$$

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

m: Total number of k-local terms

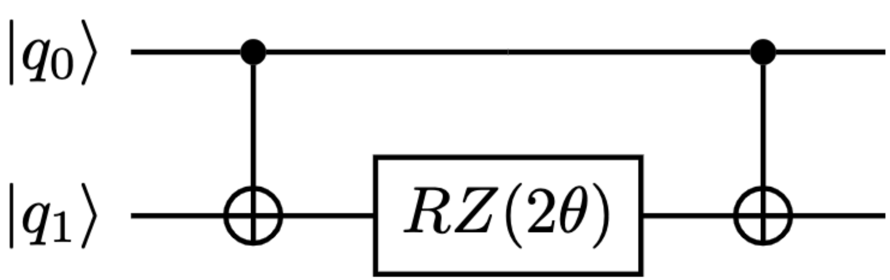
ϵ : Desired accuracy

$$\text{Total Cost } = nmC_H \sim O\left(\frac{t^2 m C_H}{\epsilon}\right)$$

Suzuki-Lie-Trotter

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

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



Suzuki-Lie-Trotter

Pauli Z's produce XOR in phases

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

So that

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

Note also

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

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

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

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

Suzuki-Lie-Trotter

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

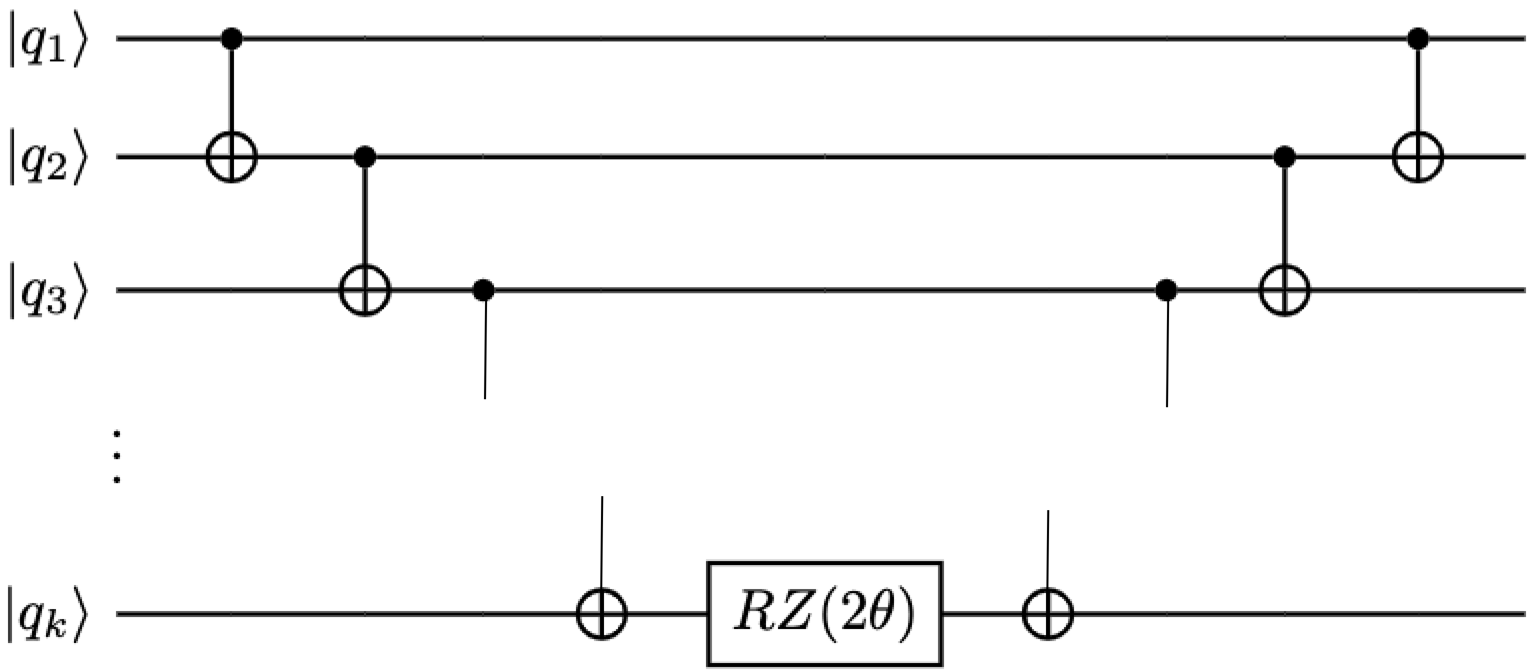
- $$\prod_{i=1}^{k-1} \mathrm{C}_i\text{-NOT}_{i+1}|b_1\rangle \ldots |b_k\rangle = |b_1\rangle|b_1 \oplus b_2\rangle \ldots |b_1 \oplus b_2 \oplus \cdots \oplus b_k\rangle$$

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

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

Suzuki-Lie-Trotter

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



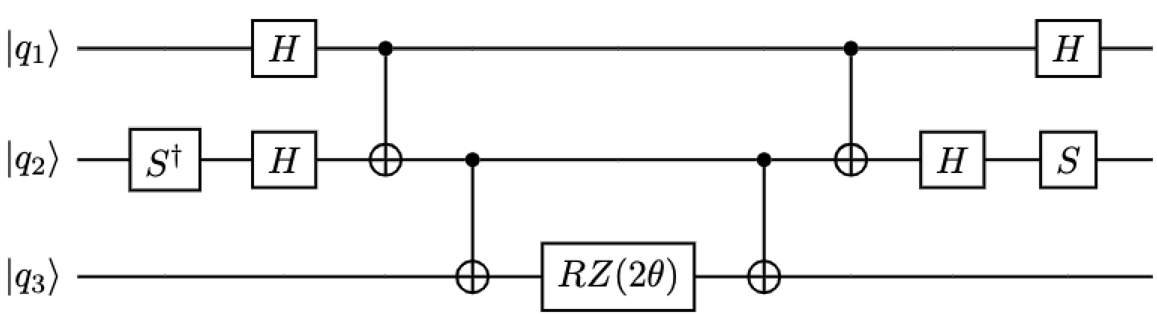
Suzuki-Lie-Trotter

Note that

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

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

E.g. $e^{-i\theta X_1 Y_2 Z_3} = \left(H \otimes (SH) \otimes I\right) e^{-i\theta Z_1 Z_2 Z_3} \left(H \otimes (SH)^{\dagger} \otimes I\right)$



Suzuki-Lie-Trotter

$$e^{-iHt} = \left(e^{-iH\Delta t}\right)^n \qquad \Delta t = t/n$$

$$e^{-iH\Delta t} \approx e^{-iH_1\Delta t} \ldots e^{-iH_m\Delta t} + O(\Delta t^2)$$

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

m: Total number of k-local terms

ϵ : Desired accuracy

$$\text{Total Cost } = nmC_H \sim O\left(\frac{t^2 mC_H}{\epsilon}\right) \sim O\left(\frac{t^2 mk}{\epsilon}\right)$$

Suzuki-Lie-Trotter

Suzuki higher-order formulas

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

yields a better approximation

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

Recursive definition

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

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

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

Suzuki-Lie-Trotter

$$\text{Total Cost} \sim \frac{(\alpha_{comm} t)^{1+\frac{1}{2k}}}{\epsilon^{\frac{1}{2k}}}$$

$$\alpha_{comm} = \max_{i,m} \left| [H_{i_1}, [H_{i_2}, \ldots [H_{i_{m-1}}, H_{i_m}]] \ldots] \right|^{1/m}$$

Linear Combination of Unitaries

Taylor series expansion

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

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

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

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

Linear Combination of Unitaries

Problem

Sum of unitaries is not unitary!

E.g. $$\frac{1}{2}(\mathbb{I} + Z) = |0\rangle\langle 0|$$

Solution

$$|0\rangle \otimes |\psi\rangle$$

Use ancillas!

Block encode non-unitary operation in a larger unitary

$$\begin{pmatrix} \tilde{V} & \cdot \\ \cdot & \cdot \end{pmatrix} \begin{pmatrix} |\psi\rangle \\ 0 \end{pmatrix} = \begin{pmatrix} \tilde{V}|\psi\rangle \\ \cdot \end{pmatrix}$$

Linear Combination of Unitaries

Given

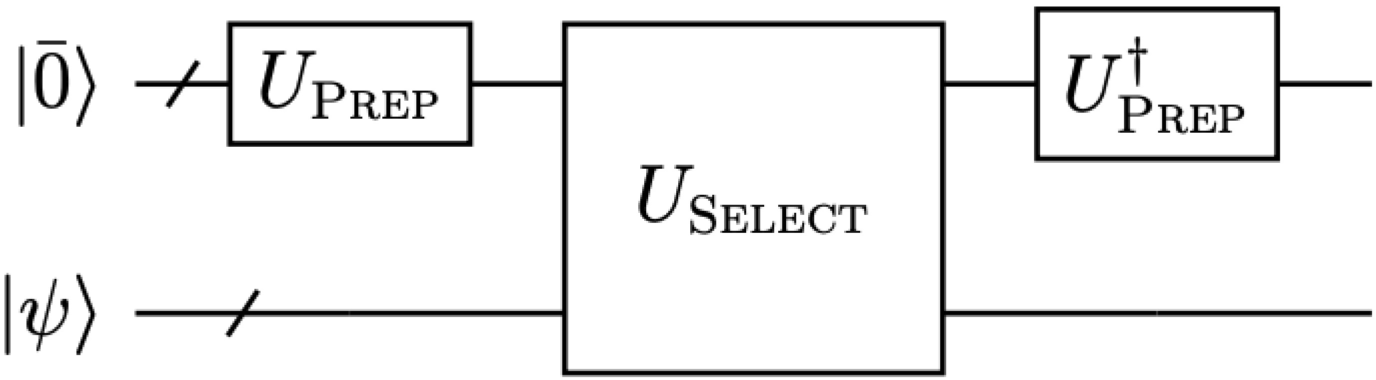
$$A = \sum_{i=1}^{L} \alpha_i U_i \qquad \alpha_i > 0$$

Construct

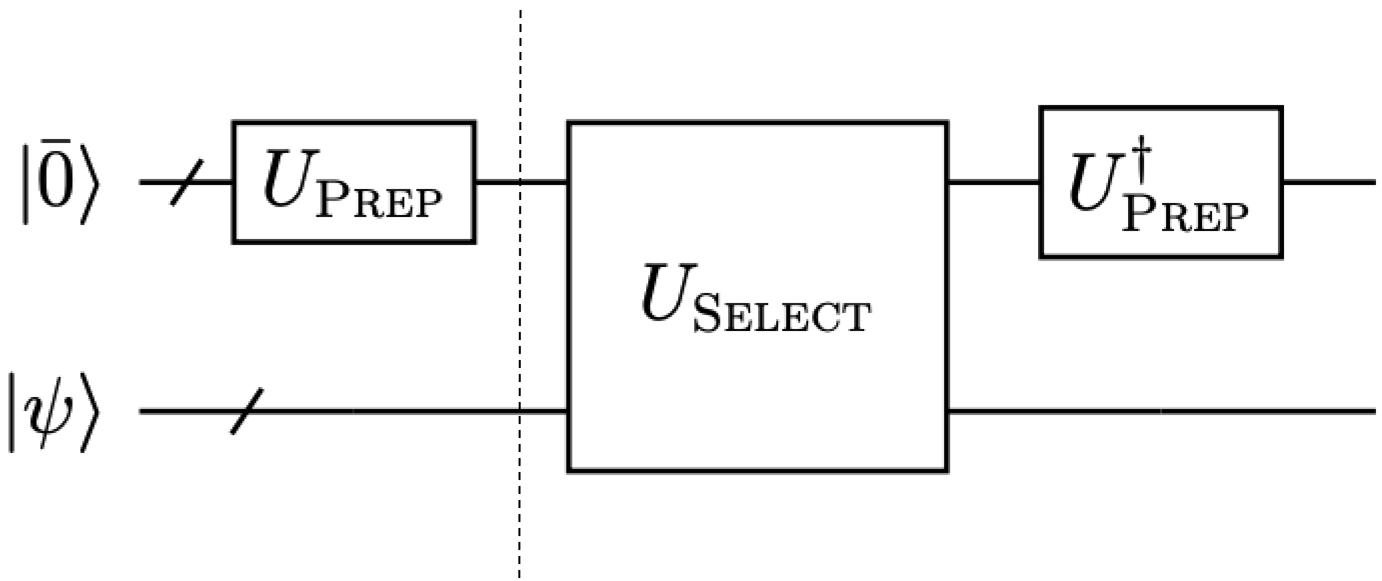
$$U_{PREP}|\bar{0}\rangle = \frac{1}{\sqrt{|\alpha|_1}} \sum_{i=1}^{L} \sqrt{\alpha_i}|i\rangle \qquad |\alpha|_1 = \sum_{i=1}^{L} \alpha_i$$

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

Linear Combination of Unitaries

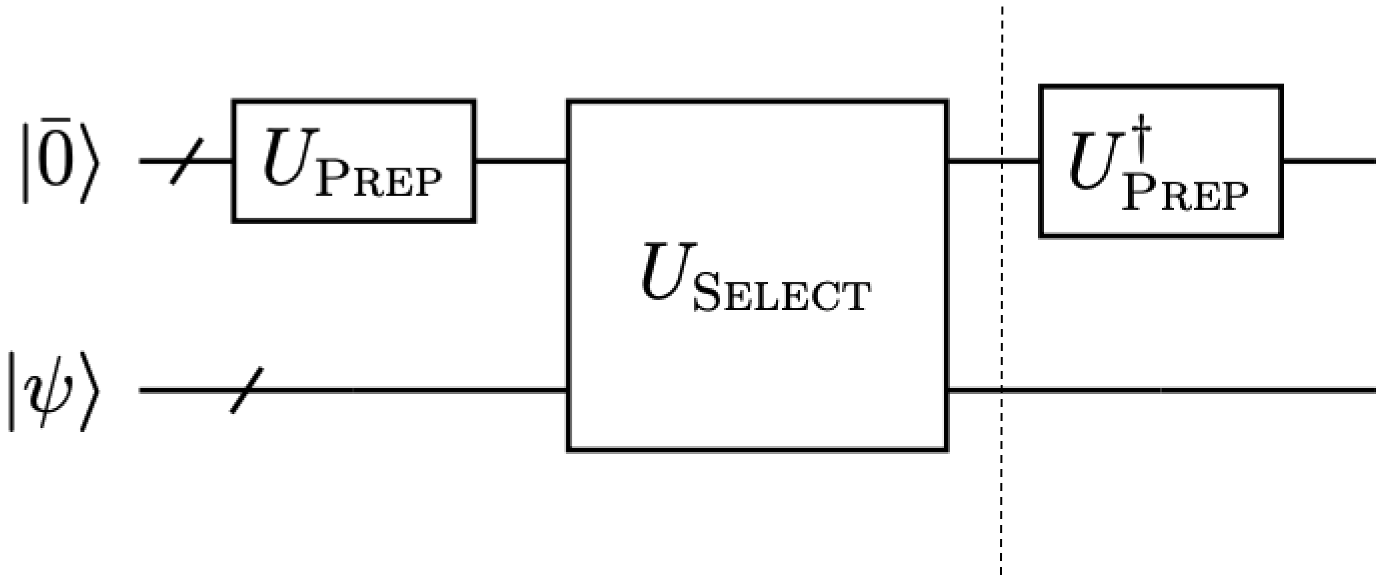


Linear Combination of Unitaries



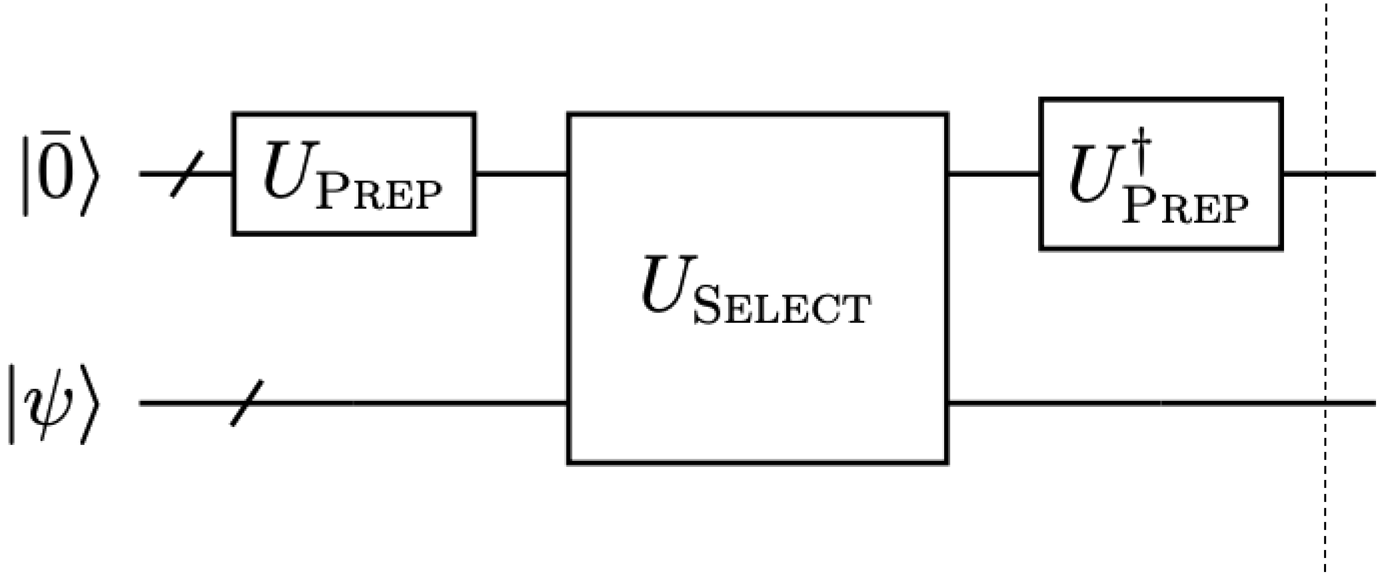
$$\left(\frac{1}{\sqrt{|\alpha|_1}} \sum_{i=1}^{L} \sqrt{\alpha_i} |i\rangle \right) \otimes |\psi\rangle$$

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 $R = 2\left(|\bar{0}\rangle\langle\bar{0}| \otimes \mathbb{I}_s\right) - \mathbb{I}$,

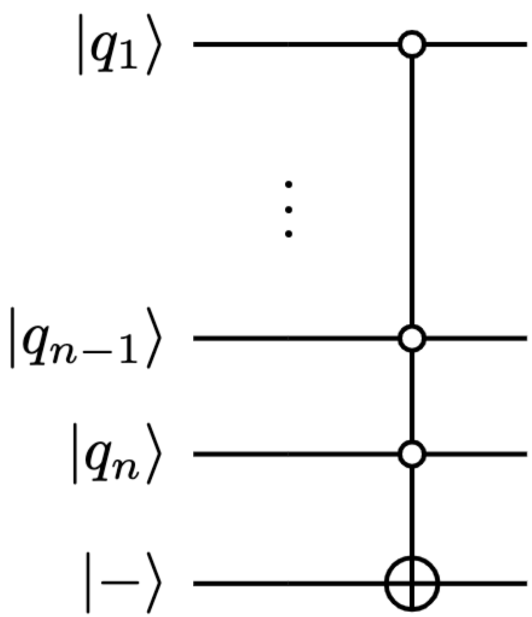
the unitary $A = WRW^{\dagger}RW$ achieves

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

Linear Combination of Unitaries

Reflection operator $R = 2|\bar{0}\rangle\langle\bar{0}| - I$

$$|\bar{0}\rangle = |0\rangle^{\otimes n}$$



$$(R \otimes \mathbb{I})\, |\bar{0}\rangle|-\rangle = |\bar{0}\rangle|-\rangle$$

$$(R \otimes \mathbb{I})\, |\bar{b}\rangle|-\rangle = -|\bar{b}\rangle|-\rangle$$

$$\langle\bar{b}|\bar{0}\rangle = 0$$

$$|-\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)$$

Linear Combination of Unitaries

Approximating a single step

$$V_r = e^{-iHt/r} \approx \sum_{k=0}^{K} \frac{1}{k!} (-iHt/r)^k = \tilde{V}_r$$

Total accuracy of all steps must be ϵ

$$K = O\left(\frac{\log(T/\epsilon)}{\log\log(T/\epsilon)}\right) \quad \Rightarrow \quad ||\tilde{V}_r - V_r|| \sim O(\epsilon/r)$$

$$T = (\alpha_1 + \cdots + \alpha_L)t$$

Linear Combination of Unitaries

$$\tilde{V}_r = \underbrace{\sum_{k=0}^{K} \sum_{l_1,\dots,l_k} \frac{(t/r)^k}{k!} \alpha_{l_1} \dots \alpha_{l_k}}_{s = 2 + O(\epsilon/r) \ \text{ for } r = \left\lceil \frac{T}{\ln 2} \right\rceil} \left((-i)^k U_{l_1} \dots U_{l_k} \right)$$

$$U_{PREP} |\bar{0}\rangle = \frac{1}{\sqrt{\mathcal{K}}} \sum_{k=0}^{K} \sum_{l_1,\dots,l_k=1}^{L} \sqrt{\frac{(t/r)^k}{k!} \alpha_{l_1} \dots \alpha_{l_k}} |k\rangle |l_1\rangle \dots |l_k\rangle$$

Linear Combination of Unitaries

$$U_{PREP}|\bar{0}\rangle = \frac{1}{\sqrt{\mathcal{K}}} \sum_{k=0}^{K} \sum_{l_1,\ldots,l_k=1}^{L} \sqrt{\frac{(t/r)^k}{k!} \alpha_{l_1} \ldots \alpha_{l_k} |k\rangle |l_1\rangle \ldots |l_k\rangle}$$

First prepare the $|k\rangle$ register with basis states $|k\rangle = |1\rangle^{\otimes k} |0\rangle^{\otimes K-k}$

$$\frac{1}{\sqrt{\mathcal{N}}} \sum_{k=0}^{K} \sqrt{\frac{(t/r)^k}{k!}} |1\rangle^{\otimes k} |0\rangle^{\otimes K-k}$$

Linear Combination of Unitaries

$$\frac{1}{\sqrt{\mathcal{N}}}\sum_{k=0}^{K}\sqrt{\frac{(t/r)^k}{k!}}|1\rangle^{\otimes k}|0\rangle^{\otimes K-k}$$

E.g. K=3

$$RY_0(\theta_0)|000\rangle = \cos(\theta_0/2)|000\rangle + \sin(\theta_0/2)|100\rangle$$

$$\xrightarrow{C_0-RY_1(\theta_1)} \cos(\theta_0/2)|000\rangle + \sin(\theta_0/2)\cos(\theta_1/2)|100\rangle + \sin(\theta_0/2)\sin(\theta_1/2)|110\rangle$$

$$\xrightarrow{C_1-RY_2(\theta_2)} \cos(\theta_0/2)|000\rangle + \sin(\theta_0/2)\cos(\theta_1/2)|100\rangle + \sin(\theta_0/2)\sin(\theta_1/2)\cos(\theta_2/2)|110\rangle + \sin(\theta_0/2)\sin(\theta_1/2)\sin(\theta_2/2)|111\rangle$$

Linear Combination of Unitaries

$$\cos(\theta_0/2) = 1/\sqrt{\mathcal{N}}$$

$$\vdots$$

$$\sin(\theta_0/2)\ldots\sin(\theta_{k-1}/2)\cos(\theta_k/2) = \left[\frac{(t/r)^k}{k!}\right]^{1/2} /\sqrt{\mathcal{N}}$$

$$0 \le k < K$$

$$\sin(\theta_0/2)\ldots\sin(\theta_K/2) = \left[\frac{(t/r)^K}{K!}\right]^{1/2} /\sqrt{\mathcal{N}}$$

Linear Combination of Unitaries

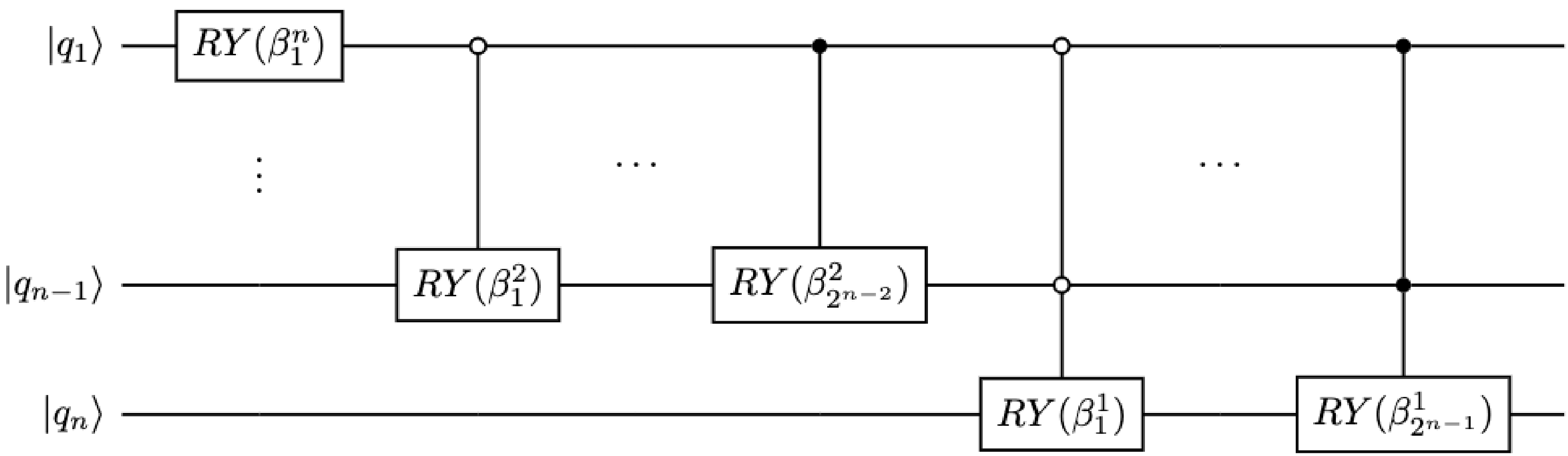
$$U_{PREP}|\bar{0}\rangle = \frac{1}{\sqrt{\mathcal{K}}} \sum_{k=0}^{K} \sum_{l_1,\ldots,l_k=1}^{L} \sqrt{\frac{(t/r)^k}{k!}\alpha_{l_1}\ldots\alpha_{l_k}} |k\rangle|l_1\rangle\ldots|l_k\rangle$$

Prepared $\frac{1}{\sqrt{\mathcal{N}}} \sum_{k=0}^{K} \sqrt{\frac{(t/r)^k}{k!}} |1\rangle^{\otimes k}|0\rangle^{\otimes K-k}$ using O(K) gates

Using O(K log L) qubits, prepare $\left(\frac{1}{\sqrt{|\alpha|_1}} \sum_{l=0}^{L-1} \sqrt{\alpha_l}|l\rangle\right)^{\otimes K}$ using O(KL log L) gates

Linear Combination of Unitaries

$$|\psi\rangle = \sum_{i=0}^{2^n-1} \alpha_i |i\rangle \qquad (L = 2^n)$$



$$\beta_j^s = 2\arcsin\left(\frac{\sqrt{\sum_{l=0}^{2^{s-1}-1} |\alpha_{(2j-1)2^{s-1}+l}|^2}}{\sqrt{\sum_{l=0}^{2^s-1} |\alpha_{(j-1)2^s+l}|^2}}\right)$$

$$\text{Cost} \sim O(L \log L)$$

Linear Combination of Unitaries

$$U_{PREP}|\bar{0}\rangle = \frac{1}{\sqrt{K}} \sum_{k=0}^{K} \sum_{l_1,\ldots,l_K=0}^{L-1} \sqrt{\frac{(t/r)^k}{k!}\alpha_{l_1}\ldots\alpha_{l_k}}|k\rangle|l_1\rangle\ldots|l_K\rangle$$

$$\tilde{V}_r = \sum_{k=0}^{K} \sum_{l_1,\ldots,l_k} \underbrace{\frac{(t/r)^k}{k!}\alpha_{l_1}\ldots\alpha_{l_k}}_{\text{"Prepare" step}} \underbrace{\left((-i)^k U_{l_1}\ldots U_{l_k}\right)}_{\text{"Select" step}}$$

"Prepare" step "Select" step

$$\text{Cost} \sim O(K L \log L)$$

Linear Combination of Unitaries

Broadly,

$$U_S = \sum_{l=0}^{L-1} |l\rangle\langle l| \otimes U_l$$

For the particular case of Taylor series approach

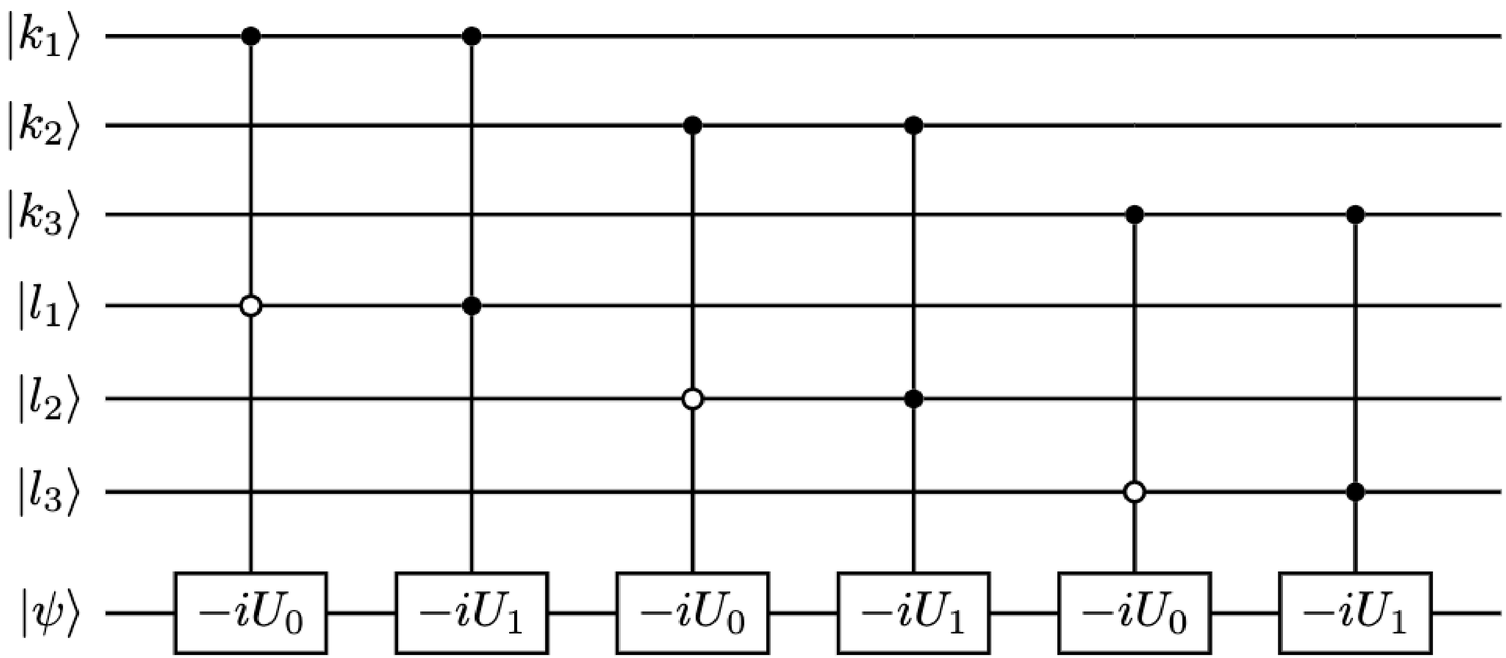
$$U_{SELECT} : |k\rangle|l_1\rangle \ldots |l_k\rangle|l_{k+1}\rangle \ldots |l_K\rangle|\psi\rangle$$
$$\rightarrow |k\rangle|l_1\rangle \ldots |l_k\rangle|l_{k+1}\rangle \ldots |l_K\rangle \left((-i)^k U_{l_1} \ldots U_{l_k}\right) |\psi\rangle$$

Implement via

$U_{S,j} : |b_j\rangle|l_j\rangle|\psi\rangle \rightarrow |b_j\rangle|l_j\rangle(-iU_{l_j})^{b_j} |\psi\rangle$ for each $j \in \{1, \ldots, K\}$

Linear Combination of Unitaries

E.g. K=3, L=2



$\text{Cost} \sim O(mKL\log L)$ $\quad$ m : locality of U's

Linear Combination of Unitaries

$$
\begin{aligned}
&\beta_0|k=0\rangle\,(\text{product state})_K\,|\psi\rangle \\
&+\beta_1|k=1\rangle\left[\sum_{l=1}^{L}|l_1\rangle\,(\text{product state})_{K-1}\,(-i\alpha_{l_1}U_{l_1})|\psi\rangle\right] \\
&+\beta_2|k=2\rangle\left[\sum_{l_1,l_2=1}^{L}|l_1\rangle|l_2\rangle\,(\text{product state})_{K-2}\,(-i)^2\alpha_{l_1}\alpha_{l_2}U_{l_2}U_{l_1}|\psi\rangle\right] \\
&+\quad\ldots \\
&+\beta_K|k=K\rangle\left[\sum_{l_1,\ldots,l_K=1}^{L}|l_1\rangle\ldots|l_K\rangle(-i)^K\alpha_{l_1}\ldots\alpha_{l_K}U_{l_K}\ldots U_{l_1}|\psi\rangle\right]
\end{aligned}
$$

Linear Combination of Unitaries

$$\text{Cost of single segment} \sim O(KL\log L)$$

$$\sim O\left(\frac{L\log L\log(T/\epsilon)}{\log\log(T/\epsilon)}\right)$$

$$\text{Total cost} \sim O(rKL\log L)$$

$$T = \left(\sum_i |\alpha_i|\right) t$$

$$\sim O\left(T\frac{L\log L\log(T/\epsilon)}{\log\log(T/\epsilon)}\right)$$

Quantum Singular Value Transform

Quantum Signal Processing

There exists a $\vec{\phi} = (\phi_0, \dots, \phi_d)$ such that

$$e^{i\phi_0 Z} \prod_{k=1}^{d} W(a) e^{i\phi_k Z} = \begin{pmatrix} P(a) & iQ(a)\sqrt{1-a^2} \\ iQ^\star(a)\sqrt{1-a^2} & P^\star(a) \end{pmatrix}$$

where $a \in [-1, 1]$ and $W(a) = \begin{pmatrix} a & i\sqrt{1-a^2} \\ i\sqrt{1-a^2} & a \end{pmatrix}$, for any polynomials P(a) and Q(a) such that

- $\deg(P) \leq d, \ \deg(Q) \leq d-1$
- *P* has parity d mod 2, and *Q* has parity (d-1) mod 2
- $|P|^2 + (1-a^2)|Q|^2 = 1$

Quantum Singular Value Transform

Quantum Eigenvalue Transform

Given a block encoding of Hamiltonian $\mathcal{H} = \sum_i \lambda_i |\lambda_i\rangle\langle\lambda_i|$

as $U = \begin{matrix} & \Pi & \\ \Pi & \left[\begin{matrix} \mathcal{H} & \cdot \\ \cdot & \cdot \end{matrix}\right] \end{matrix}$, given conditional phase shift $\Pi_\phi = e^{i\phi(2\Pi - I)}$

$$U_{\vec{\phi}} = \begin{matrix} & \Pi & \\ \Pi & \left[\begin{matrix} \mathrm{Poly}(\mathcal{H}) & \cdot \\ \cdot & \cdot \end{matrix}\right] \end{matrix} = \begin{cases} \left[\prod_{k=1}^{d/2} \Pi_{\phi_{2k-1}} U^\dagger \Pi_{\phi_{2k}} U\right] & \text{even } d \\ \Pi_{\phi_1} U \left[\prod_{k=1}^{(d-1)/2} \Pi_{\phi_{2k}} U^\dagger \Pi_{\phi_{2k+1}} U\right] & \text{odd } d \end{cases}$$

$$\mathrm{Poly}(\mathcal{H}) = \sum_\lambda \mathrm{Poly}(\lambda)|\lambda\rangle\langle\lambda|$$

$(\mathrm{Poly}(\lambda)$ has degree $d)$

Quantum Singular Value Transform

Explicit example

$$U = \begin{bmatrix} \mathcal{H} & \sqrt{I - \mathcal{H}^2} \\ \sqrt{I - \mathcal{H}^2} & -\mathcal{H} \end{bmatrix}$$

$$\mathcal{H} = \langle 0 | U | 0 \rangle$$

$$U = Z \otimes \mathcal{H} + X \otimes \sqrt{I - \mathcal{H}^2}$$

with action

$$U|0\rangle|\lambda\rangle = \lambda|0\rangle|\lambda\rangle + \sqrt{1-\lambda^2}|1\rangle|\lambda\rangle$$
$$U|1\rangle|\lambda\rangle = -\lambda|1\rangle|\lambda\rangle + \sqrt{1-\lambda^2}|0\rangle|\lambda\rangle$$

Quantum Singular Value Transform

Explicit example

$$U = \begin{bmatrix} \mathcal{H} & \sqrt{I - \mathcal{H}^2} \\ \sqrt{I - \mathcal{H}^2} & -\mathcal{H} \end{bmatrix}$$

$$\begin{aligned} U &= \sum_\lambda \begin{bmatrix} \lambda & \sqrt{1 - \lambda^2} \\ \sqrt{1 - \lambda^2} & -\lambda \end{bmatrix} \otimes |\lambda\rangle\langle\lambda| \\ &= \sum_\lambda \left[\sqrt{1 - \lambda^2} X + \lambda Z\right] \otimes |\lambda\rangle\langle\lambda| \\ &=: \sum_\lambda R(\lambda) \otimes |\lambda\rangle\langle\lambda| = \bigoplus_\lambda R(\lambda) \end{aligned}$$

$\mathcal{H}$ has been "qubitized"

Quantum Singular Value Transform

But we can also construct $\mathcal{H}/|\alpha|_1 = (1/|\alpha|_1)\sum_i \alpha_i H_i = \langle g|U|g\rangle$

using the operators we constructed for LCU!

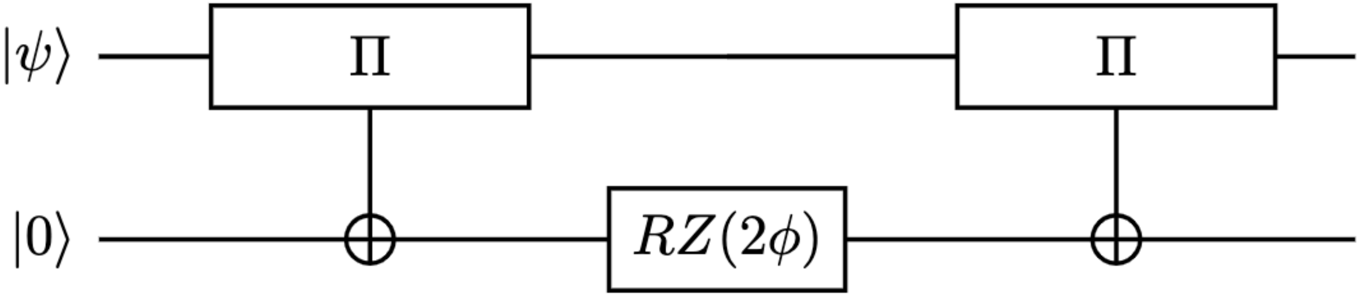
$$|g\rangle = U_{PREP}|\bar{0}\rangle = \frac{1}{\sqrt{|\alpha|_1}}\sum_i \sqrt{\alpha_i}|i\rangle$$

and

$$U = U_{SELECT} = \sum_i |i\rangle\langle i| \otimes H_i$$

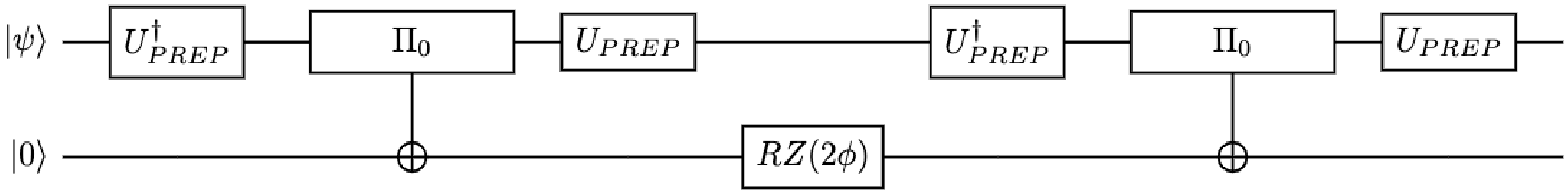
Quantum Singular Value Transform

$$\Pi_\phi = e^{i\phi(2\Pi - I)} = e^{i\phi}|g\rangle\langle g| + e^{-i\phi}|g^\perp\rangle\langle g^\perp|$$



Quantum Singular Value Transform

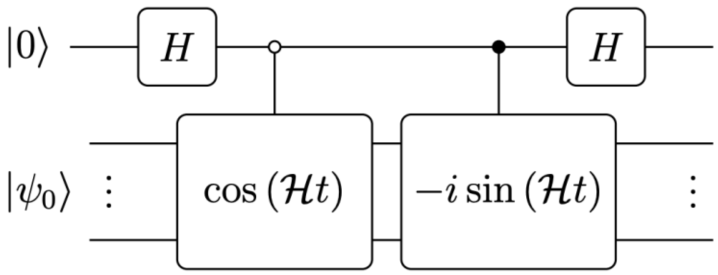
$$\Pi_\phi = e^{i\phi(2\Pi - I)} = U_{PREP}\left(e^{i\phi}|0\rangle\langle 0| + e^{-i\phi}|0^\perp\rangle\langle 0^\perp|\right)U_{PREP}^\dagger$$



Quantum Singular Value Transform

Hamiltonian simulation

$$e^{-i\mathcal{H}t} = \cos(\mathcal{H}t) - i\sin(\mathcal{H}t)$$



Jacobi-Anger expansion

$$\cos(xt) = J_0(t) + 2\sum_{k=1}^{\infty}(-1)^k J_{2k}(t) T_{2k}(x)$$

$$\sin(xt) = 2\sum_{k=0}^{\infty}(-1)^k J_{2k+1}(t) T_{2k+1}(x)$$

$J_i(x)$: Bessel function of order i

$T_i(x)$: Chebyshev polynomial of order i

Quantum Singular Value Transform

Jacobi-Anger expansion

$$\cos(xt) = J_0(t) + 2\sum_{k=1}^{\infty}(-1)^k J_{2k}(t) T_{2k}(x)$$

$$\sin(xt) = 2\sum_{k=0}^{\infty}(-1)^k J_{2k+1}(t) T_{2k+1}(x)$$

To achieve accuracy $O(\epsilon)$, truncate at 2k' and 2k'+1 respectively, where

$$k' \sim \text{Query complexity} \sim O\left(|\alpha|_1 t + \frac{log(1/\epsilon)}{log\frac{log(1/\epsilon)}{|\alpha|_1 t}}\right)$$

Summary

Costs

Trotterization $$O\left(\frac{(\alpha_{comm}t)^{1+\frac{1}{2k}}}{\epsilon^{\frac{1}{2k}}}\right)$$

LCU $$O\left(|\alpha|_1 t\frac{L\log L\log\left(T/\epsilon\right)}{\log\log\left(T/\epsilon\right)}\right)$$

QSVT $$O\left(|\alpha|_1 t+\frac{log(1/\epsilon)}{log\frac{log(1/\epsilon)}{|\alpha|_1 t}}\right)$$

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Thank you!

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Extra slides

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

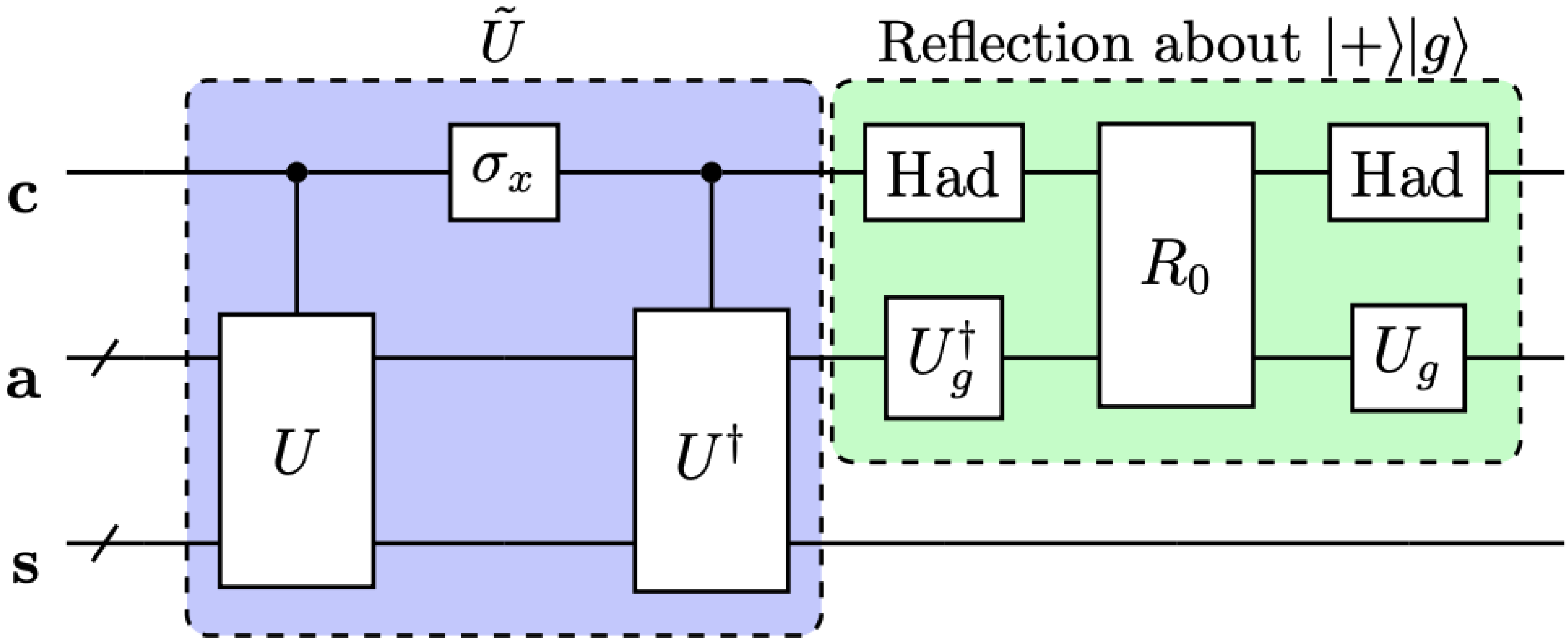
We can construct $H = \langle g|U|g\rangle$

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

from the LCU construction.

Qubitization

Circuit for W_U



$U = U_{SELECT}$ $\quad$ $U_g = U_{PREP}$

Qubitization

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

defines an LCU algorithm using W_U, which has been decomposed into a direct sum of 2-dimensional subspaces, i.e. has been "qubitized"

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