Quantum algorithms for Dynamics Simulation: Hamiltonian Simulation and Linear Differential Equations

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Outline

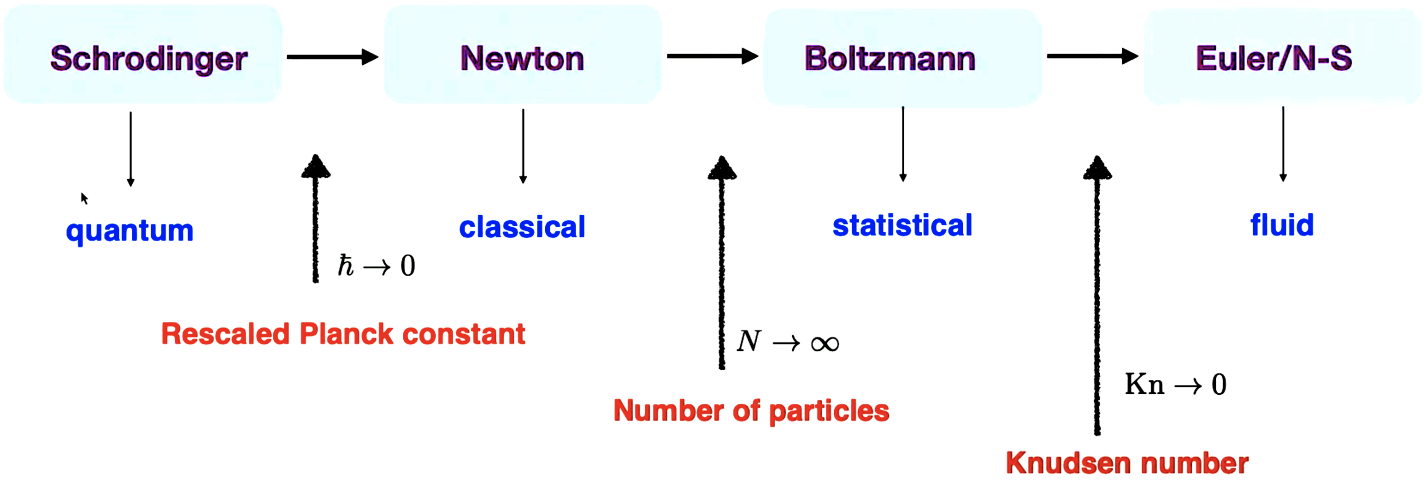
1. Hamiltonian Simulation Problem
   - Motivations
   - Expected cost
2. Hamiltonian Simulation Algorithms
   - Trotterization
   - Block-encoding, Truncated Taylor series, Optimal Ham Sim by QSVT

Part 1: Hamiltonian Simulation (time-independent case)

Different Levels of Physics

multiscale physics fig by Prof. Qin Li

Different Levels of Physics



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Schrödinger equation for Molecular Dynamics

To describe its behaviour: (x: nuclei coordinates, y: electronic coordinates, M : mass of a nucleus, m: mass of an electron.)

$$\hat{H}_{\text{total}} = \frac{\sim^2}{2M} \text{ x } \frac{\sim^2}{2m} \text{ y} + V(x;y); \quad x \; 2 \; R^d; y \; 2 \; R^n$$

$$i\sim @ = \hat{H}_{\text{total}}$$

Quantum Computing 101

"... 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."

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$$i\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle; \quad |\psi(0)\rangle = |\psi_0\rangle:$$

To simulate $\mathcal{T}e^{-i\int_0^t H(s)\,ds}$ for H of very high dimension!

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Examples of H : many-body Hamiltonian

$$H = \sum_{E \in S\{I,X,Y,Z\}^n} {}_E E;$$

k-local Hamiltonian (TFIM, Heisenberg models, etc), etc.

Error Metrics: Speci c case v.s. Worst case

Taking into account initial conditions : consider vector norm, instead of operator norm.

$$U_{app}\,|\,_0\rangle \quad e^{\ iHt}\,|\,_0\rangle \qquad U_{app} \quad e^{\ iHt} \qquad :$$

[Sahinoglu-Somma 2021], [An-Fang-Lin 2020], [Tres-Fang 2022], [BornsWeil-Fang 2022], [Zhao-Zhou-Shaw-Li-Childs 2022], etc

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$$U_{app}^{y} O U_{app} \quad e^{iHt}\, O e^{\ iHt}$$

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Taking into account both and consider observable expectation $|\langle\ _0|\, U_{app}^{y} O U_{app}\,|\ _0\rangle \quad \langle\ _0|\, e^{iHt}\ Oe^{\ iHt}\,|\ _0\rangle|$

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Speci c case v.s. Worst case: Take-away

"Spectrum" of various error measurements:

Observable expectation

Vector norm

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[1] The cost can be improved for product formulas.

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Speci c case v.s. Worst case

Taking into account the speci c instance, the error (and hence the cost) can be improved. [1]

In this lecture, we only focus on the worst case, i.e. error in the operator norm of unitaries.

[1] The cost can be improved for product formulas.

Expected Complexity?

[2] [Feymann 1985]

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No-fast-forwarding Theorem: (informal)
Simulating Hamiltonian dynamics for time t requires complexity (t).

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(Any Classical Alg. under reasonable complexity conjectures)

Hamiltonian Simulation is BQP-hard.
(Any quantum circuit can be efficiently implemented by the dynamics of a local Hamiltonian. [2])

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Hamiltonian Simulation Algorithms

Trotterization (= Product Formulae = Time/Operator Splitting)

1st-order Trotter formula (Lie-Trotter) for $H = H_1 + H_2$

$$e^{iHt} \qquad e^{iH_2 t/L} e^{iH_1 t/L}{}^{L}$$

Cost/Complexity?

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$$e^{iHt} \approx \left(e^{iH_2 t/L} e^{iH_1 t/L} \right)^L$$

Cost/Complexity? error estimate and circuit implementation

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$$e^{iHt} = e^{iH_2 t/L} e^{iH_1 t/L}{}^{L} + O\left(k[H_1; H_2]kt^2/L\right)$$

The number of Trotter steps $L = O\left(k[H_1; H_2]kt^2/\right.$

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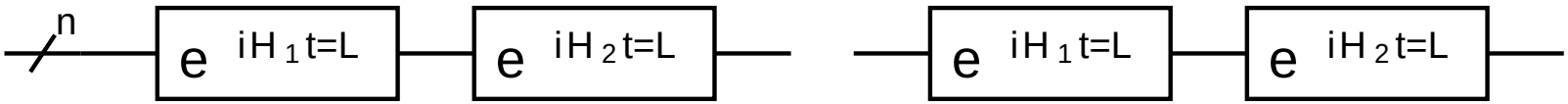

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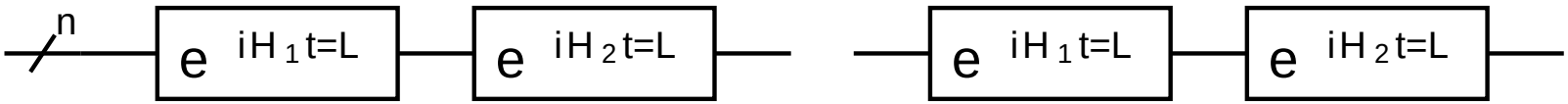

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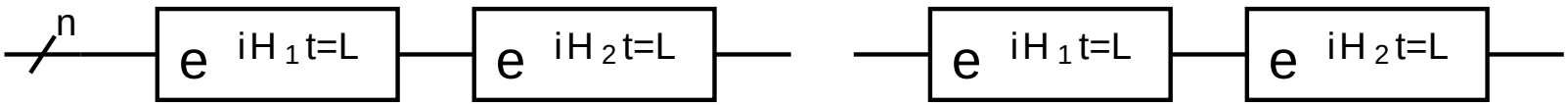

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High order (p-th): query complexity $O\left({}_H t^{1+1/p}/\right.{}^{1/p}$.

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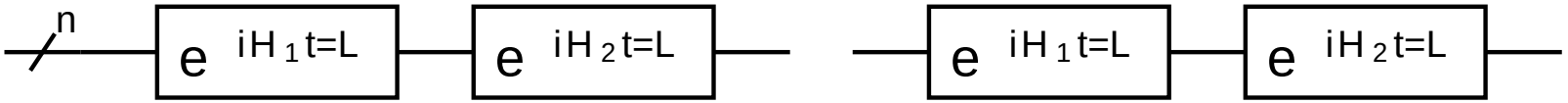

High order (p-th): query complexity $O\left(\|H\| t^{1+1/p}\right)$ [3]

Everything is unitary! No ancilla needed.

But it needs $e^{iH_j s}$ ef ciently implementable.

[3] [Suzuki 91], [Descombes-Thalhammer 2010], [Childs-Su-et Al. 2021]

[4] truncated Taylor [Berry-Childs-Cleve-Kothari-Somma 2015], QSP/QSVT [Low-Chuang 2016 and 2017], [Gilyen-Su-Low-Wiebe 2019]

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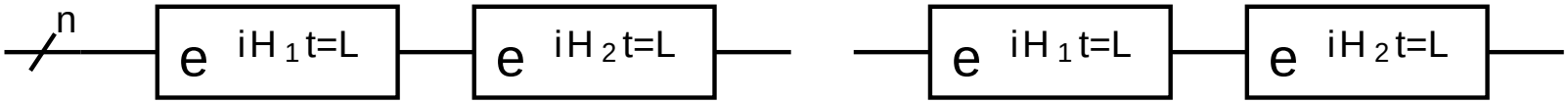

High order (p-th): query complexity $O\left(\|H\| t^{1+1=p} = \right)^{1=p}$.

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Post-Trotter, e.g., truncated Taylor series, quantum signal processing (QSP), quantum singular value transformation (QSVT) [3], etc.

$$e^{iHt} \quad \sum_{k=0}^{K} \frac{(iHt)^k}{k!} = \sum_{k=0}^{K} \sum_{\ell_1, \ldots, \ell_k} \frac{(it)^k}{k!} H_{\ell_1} H_{\ell_2} \cdots H_{\ell_k} :$$

Upshot:) O (t log(t=))

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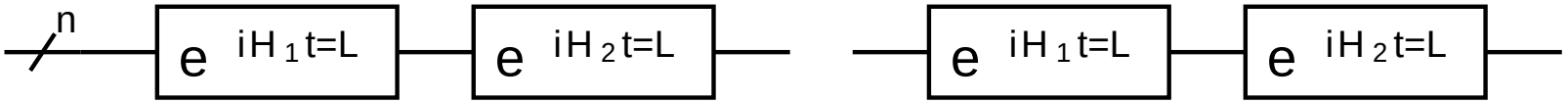

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Upshot:) $O(t \log(t=))$) Even better, say, $O(t + \log(1=))$?

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Block-Encoding – De nition

Let A be a general $2^n \quad 2^n$ matrix.

Idea:

$$U_A = \quad A \qquad \text{! ancilla qubits}$$

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$$U_A = \begin{pmatrix} \frac{A}{\alpha} & \cdot \\ \cdot & \cdot \end{pmatrix}$$

! ancilla qubits;

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$\tilde{A}$ A

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Block-Encoding – De nition

Let A be a general $2^n \quad 2^n$ matrix. kAk

Idea:

$$U_A = \begin{matrix} 0 & 1 \\ \tilde{A} & \\ @ & A \end{matrix} \qquad \tilde{A} \quad A$$

$$! \quad m \text{ ancilla qubits;}$$

De nition (Block-encoding)

U_A is an $(\ ; m; \quad)$-block-encoding of A, if

$$kA \qquad (h0^m j \quad I_n) U_A (j0^m i \quad I_n) k \qquad ;$$

for some $k \ Ak$, $m > 0$ and > 0. Here is called the subnormalization factor and m is the number of ancilla qubits, and n is the number of system qubits. When $= 0$, it is also called an $(\ ; m \ )$-block-encoding.

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Understanding: $U_A : 2^{m+n} \quad 2^{m+n}$.

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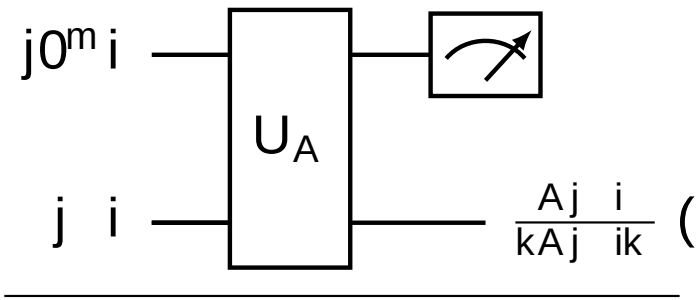
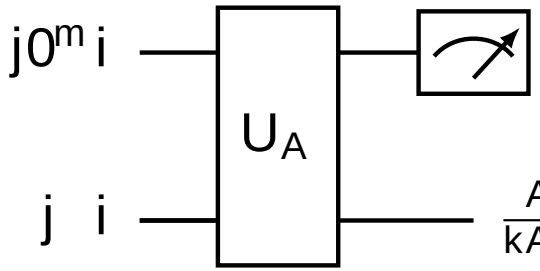


$$\frac{A j \ i}{kA j \ ik}$$ (upon getting 0 in measurement)

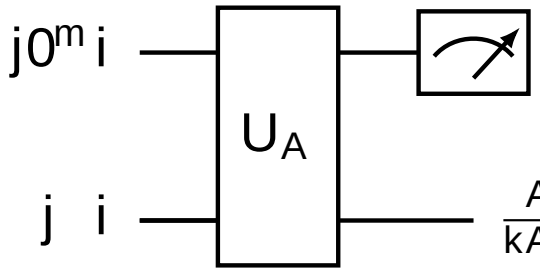
Block-Encoding – De nition cont'd



$\frac{A|\psi\rangle}{\|A|\psi\rangle\|}$ (upon getting 0 in measurement)

$$|0\rangle\langle 0| \otimes \tilde{A} + |1\rangle\langle 1| \otimes \tilde{A}; \quad |\psi\rangle = \begin{pmatrix} |\psi\rangle \\ 0 \end{pmatrix}; \quad U_A|0\rangle|\psi\rangle = \begin{pmatrix} \tilde{A}|\psi\rangle \\ 0 \end{pmatrix} + |\Phi\rangle\langle 1|:$$

Block-Encoding – De nition cont'd



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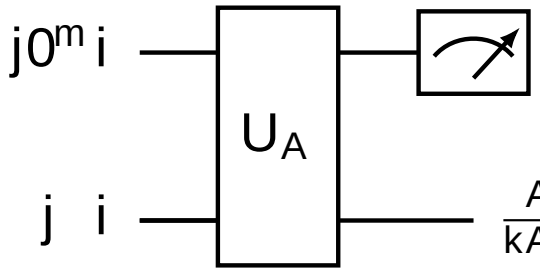
$$|0\rangle\langle 0| \otimes \tilde{A} + |1\rangle\langle 1| \otimes \tilde{A}$$

$$|0\rangle\langle 0| \otimes \tilde{A}|\psi\rangle = \begin{cases} |0\rangle|\psi\rangle, \\ |0\rangle\tilde{A}|\psi\rangle. \end{cases}$$

Question: Well-de ned? Not an empty set?

Block-Encoding – De nition cont'd



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$$|0\rangle\langle 0| \otimes \tilde{A} + |1\rangle\langle 1| \otimes \tilde{A}; \quad U_A|0\rangle|\psi\rangle = \alpha\left|0\right\rangle\tilde{A}|\psi\rangle + \left|1\right\rangle|\psi_0^\perp\rangle$$

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Trivial example (unitary): U is a $(1; 0; 0)$-block-encoding of U.

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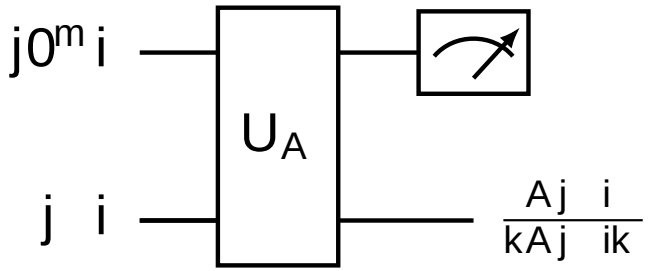


(upon getting 0 in measurement)

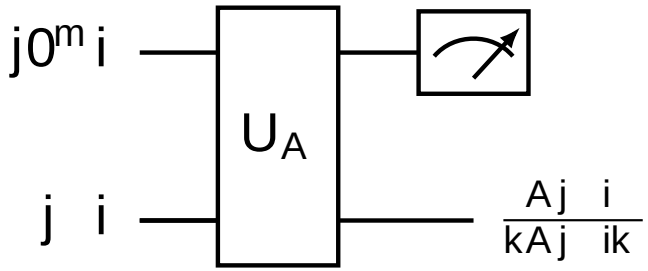
$$|0\rangle|\psi\rangle = |0\rangle|\psi\rangle = \begin{matrix}|0\rangle|\psi\rangle \\ |1\rangle|\psi\rangle\end{matrix}; \quad U_A|0\rangle|\psi\rangle = \begin{matrix}\tilde{A}|0\rangle|\psi\rangle \\ |1\rangle|\psi\rangle\end{matrix} = \tilde{A}|0\rangle|\psi\rangle + |1\rangle|\psi\rangle:$$

Question: Well-de ned? Not an empty set?

Trivial example (unitary): U is a $(1; 0; 0)$-block-encoding of U.

$(; 1)$-block-encoding is general. WLOG, assume $\|A\| \quad 1$.

Block-Encoding – De nition cont'd



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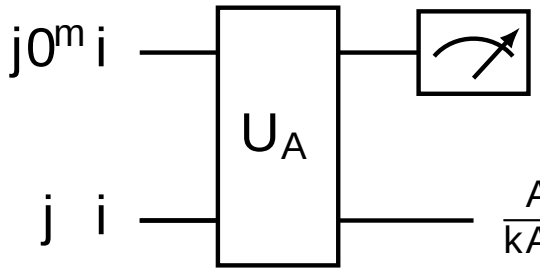

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Proof: $A = W \quad V^y$. All singular values $2\ [0;1]$.

$$U_A := \begin{pmatrix} W & 0 \\ 0 & I_n \end{pmatrix} \begin{pmatrix} A & \sqrt{I_n - AA^\dagger} \\ \sqrt{I_n - A^\dagger A} & -A^\dagger \end{pmatrix} \begin{pmatrix} V^y & 0 \\ 0 & I_n \end{pmatrix}$$

$$= \begin{pmatrix} A & W\sqrt{I_n - A^\dagger A} \\ \sqrt{I_n - AA^\dagger}\,V^y & \end{pmatrix}$$

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Sparse Input Model

Question: Ef cient to construct?

[Gilyen-Su-Low-Wiebe 2018], see also [Berry-Childs 2012], [Low-Chuang 2017]

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Upshot: sparse matrix (Hamiltonian) is ok!

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Sparse Input Model

Question: Ef cient to construct?

Upshot: sparse matrix (Hamiltonian) is ok!

We assume that H is a s-sparse matrix with kHk_{max} 1. The information of H is given through the following oracles:

$$\begin{aligned} U_{row}\ jj;s\,i &= jj;\ row(j;s)i\ ; \\ U_{col}\ jj;s\,i &= jj;\ col(j;s)i\ ; \\ U_{val}\ jj;k;z\,i &= jj;k;z\quad H_{jk}\ (t)i\ : \end{aligned} \tag{1}$$

Here $row(j;s)$ is the row index of the sth nonzero element in the j th column, $col(j;s)$ is the column index of the sth nonzero element in the j th row.

A $(s;n+3;\ )$-block-encoding of H can be constructed via $O(1)$ queries to above oracles and $O(n+\log^{5=2}(s=\ )$ primitive gates.

[Gilyen-Su-Low-Wiebe 2018], see also [Berry-Childs 2012], [Low-Chuang 2017]

Block-Encoding – Properties

Properties: Let U_A be an $(\ ; a; \ )$-BE of A; U_B be a $(\ ; b; \ )$-BE of B

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Proof:

$$AB \qquad (\langle 0|^{a+b} \quad I)(I_b \quad U_A)(I_a \quad U_B)(|0\rangle^{a+b} \quad I)$$

$$= AB \qquad \underbrace{(\langle 0|^{a} \quad I)U_A(|0\rangle^{a} \quad I)}_{A} \underbrace{(\langle 0|^{b} \quad I)U_B(|0\rangle^{b} \quad I)}_{B}$$

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$$= AB \quad \tilde{A}B + \tilde{A}B \quad \tilde{A}\tilde{B} = (A \quad \tilde{A})B + \tilde{A}(B \quad \tilde{B})$$

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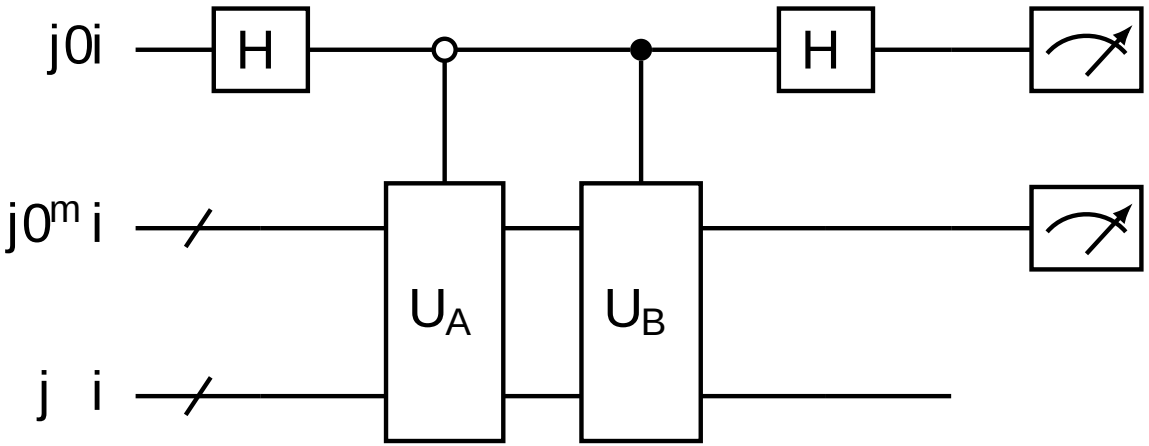
The following circuit constructs a $(2; m;\ +\ )$-BE of $A + B$.



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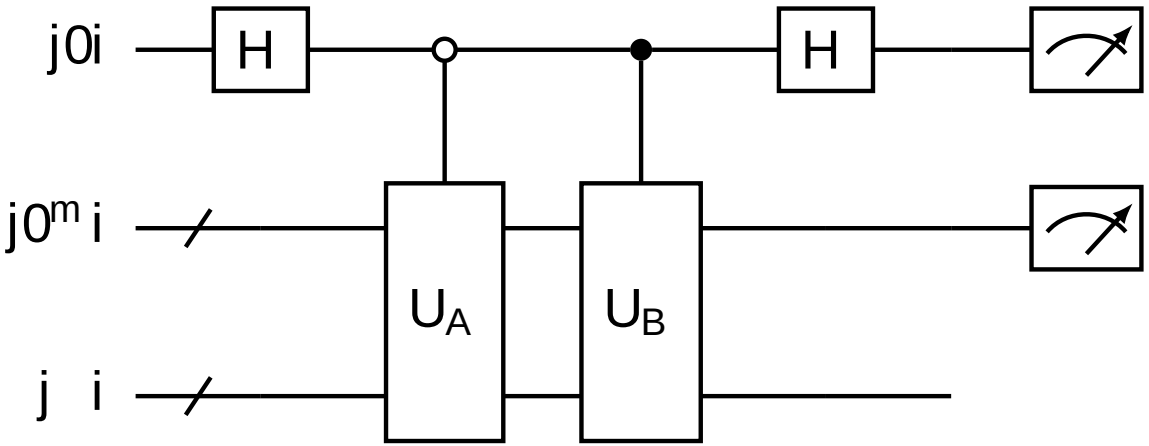

More generally, linear combination of block-encodings can be constructed via Linear Combination of Unitaries (LCU) Lemma.

LCU Lemma

LCU Lemma: $T = \sum_{j \in [L]} c_j U_j$ for unitaries U_j. $\|c\|_1 = \sum_{j \in [L]} |c_j|$.

LCU [Berry-Childs-Kothari 2015], General LCBE [Gilyen-Su-Low-Wiebe 2018]

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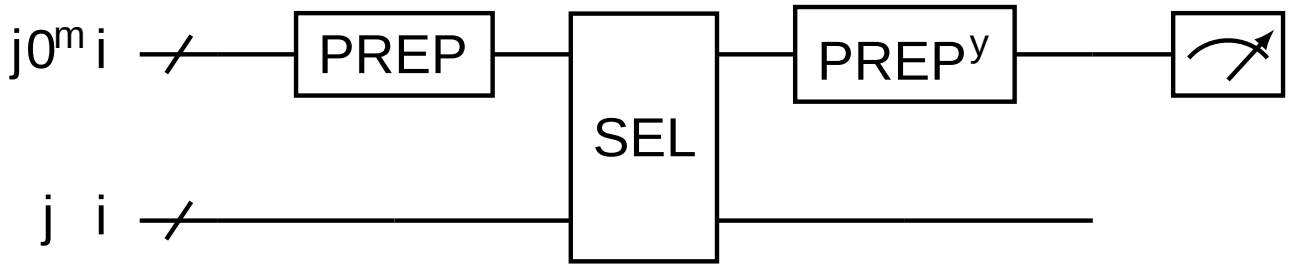
One can get a $(\|c\|_1, \lceil \log_2 L \rceil)$-block-encoding by:

$$\mathrm{SEL} := \sum_{j \in [L]} |j\rangle\langle j| \otimes U_j$$

$$\mathrm{PREP}\,|0\rangle = \frac{1}{\sqrt{\|c\|_1}} \sum_{j \in [L]} \sqrt{c_j}\,|j\rangle.$$



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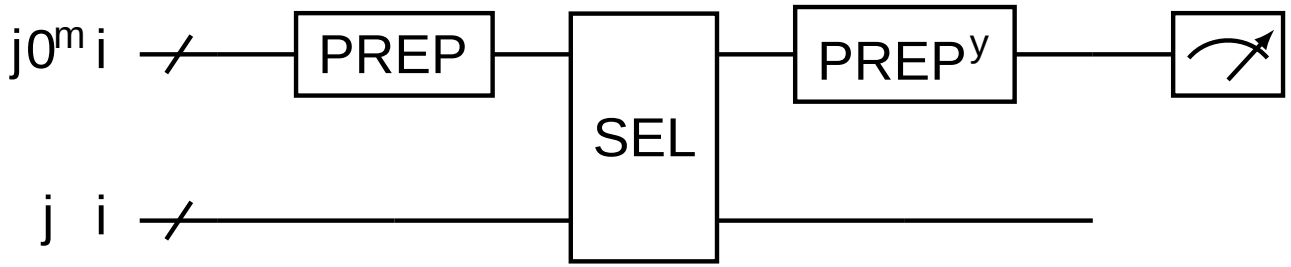

General LCBE: $\max_j m_j + \lceil \log_2 L \rceil$ ancillas

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Matrix Function and Truncated Taylor series

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Truncated Taylor Series kHk .

$$e^{iH\ t} \quad \sum_{k=0}^{K} \frac{(\ iH\ \ t)^k}{k!} = \sum_{k=0}^{K} \sum_{`_1;\ \ ;`_k} \frac{(\ i\ \ t)^k}{k!} H_{`_1} H_{`_2} \quad H_{`_k} :$$

Number of time steps $L = t= \ t = O(\ t\ ); K = O(\frac{\log(\ t= \ )}{\log\log(\ t= \ )})$

) Query Complexity: $O(\ t\ \frac{\log(\ t= \ )}{\log\log(\ t= \ )})$.

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Number of time steps $L = t = t = O(t); K = O\left(\frac{\log(t=)}{\log\log(t=)}\right)$

) Query Complexity: $O\left(t \frac{\log(t=)}{\log\log(t=)}\right)$.

But $A + A^2 + \cdots + A^d$
Number of ancillas: $m; 2m; \ldots; dm$) $dm + \log(d)$ HUGE!

Question: Can we do better?

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Question: Can we do better? Yes! 1 additional ancilla is suf cient!

Quantum Singular Value Transformation (QSVT) / Quantum Signal Processing (QSP)

QSVT

$A = W \quad V^{y} \quad f \ (A) := W f \ (\ ) \ V^{y}$ Generalized Matrix Function

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Theorem (QSVT with odd real polynomial)

Let U_A be a $(1; m)$-block-encoding of $A \ 2 \ C^{2^n} \quad ^{2^n}$. Given an odd polynomial $P_{<} \ (x) \ 2 \ R[x]$ of odd degree d satisfying

$$jP_{<} \ (x)j \ 6 \ 1; 8x \ 2 \ [\quad 1; 1]:$$

We can nd a sequence of phase factors $\quad 2 \ R^{d+1}$ and construct a $(1; m + 1)$ -block-encoding of $P_{<} \ (A)$ that uses $U_A \ ; U_A^{y}$, m-qubit controlled NOT, and single qubit rotation gates for $O(d)$ times.

QSVT

A = W V^y f (A) := W f ( ) V^y Generalized Matrix Function

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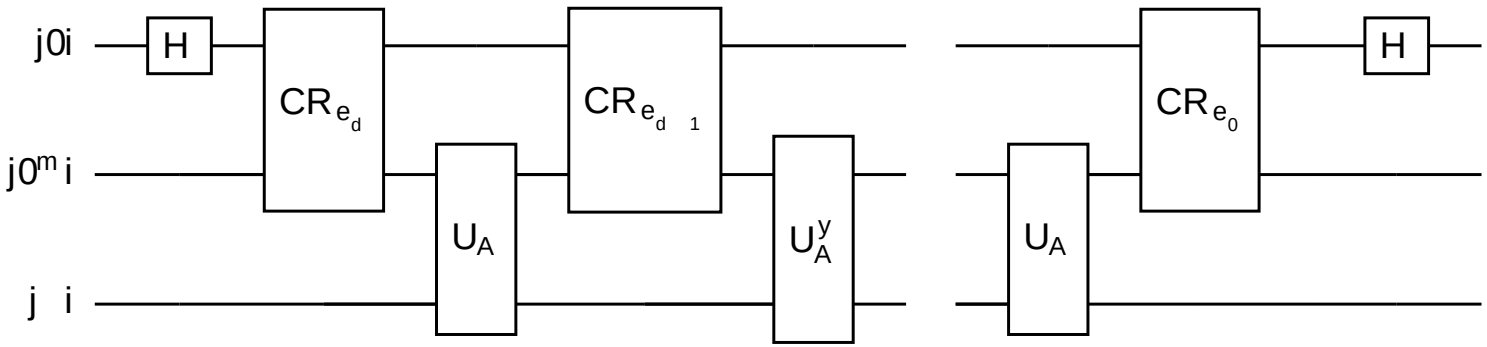

QSVT (Hermitian matrix + arbitary parity)

Theorem (QSVT for Polynomial eigenvalue transformation)

Let U_A be a $(; m;)$-block-encoding of a Hermitian matrix $A \; 2 \; C^{2^n \quad 2^n}$. Given a d-degree polynomial $P_<(x) \; 2 \; R[x]$ satisfying

$$jP_<(x)j \; 6 \; 1=2; 8x \; 2 \; [\quad 1; 1]:$$

Then for $\quad 0$, there is a quantum circuit that constructs a $(1; m + 2; 4d\sqrt{\quad = \quad + \quad})$-block-encoding of $P_<(A= \quad)$ that uses a single application of controlled-U_A, and d applications of $U_A; U_A^y$, and $O((m + 1) d)$ other one- and two-qubit gates.

Optimal Hamiltonian Simulation by QSVT

Given U_H : an (; m; 0)-block-encoding of H .
Goal: an algorithm that makes $O(t + \log(1/))$ queries to U_H .

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Jacobi-Anger expansion on $[1; 1]$:

$$\cos(tx) = J_0(t) + 2 \sum_{k=1}^{1} (1)^k J_{2k}(t) T_{2k}(x);$$

$$\sin(tx) = 2 \sum_{k=0}^{1} (1)^k J_{2k+1}(t) T_{2k+1}(x):$$

$J (t)$ denotes Bessel functions of the rst kind.

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This series converges rapidly. Truncating it with

$$r = \quad t + \frac{\log(1=)}{\log(e + \log(1 =)=t)}$$

terms gives a polynomial approximation (with precision and degree $2r + 1$) of $\cos(tx) + i \sin(tx) = e^{itx}$.

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Query Complexity: (k H k.)

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We now have block-encodings of both cos(tH) and i sin(tH) and use LCU.

[4] [Berry-Childs-Cleve-Kothari-Somma 2014/2015]

Optimal Hamiltonian Simulation by QSVT cont'd

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We now have block-encodings of both $\cos(tH)$ and $i \sin(tH)$ and use LCU. Or equivalently, directly use QSVT for polynomial eigenvalue transformation with arbitrary parity. We have a $(1; m + 2 ; \ =6)$ of $e^{itH} \ =2$.

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Optimal Hamiltonian Simulation by QSVT cont'd

Given U_H : an (; m; 0)-block-encoding of H .
Goal: an algorithm that makes $O(t + \log(1/\epsilon))$ queries to U_H .

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Last step: We want to turn e^{itH} =2 to e^{itH} .

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Oblivious Amplitude Ampli cation (OAA) [4]

Given a block-encoding U_A of A (and A is close to unitary): $A = \quad (h0j_m \quad I_n)U_A(j0i_s \quad I_n)$. De ne $R := I_m \quad 2j0i_m \ h0j_m$ and

$$W = \quad U_A(R \quad I_n)U_A^y(R \quad I_n)U_A :$$

$$(h0j_m \quad I_n)W(j0i_m \quad I_n) = \frac{3}{-}A \quad \frac{4}{3}AA^yA \quad (\frac{3}{-} \quad \frac{4}{3})A:$$

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Summary of Hamiltonian Simulation

Hamiltonian simulation: motivation; set-up

Expected cost: No-fast-forwarding theorem and BQP-hardness

Algorithms

- Trotterization
- Revisit of Block-encoding; truncated Taylor series
- Optimal Hamiltonian Simulation via QSVT

Summary of time-independent Ham Sim cont'd

- Trotterization:
  1st-order Trotter formula

$$e^{iHt} = \left(e^{iH_1 t/L} e^{iH_2 t/L}\right)^L + O(k[H_1, H_2]kt^2/L)$$

  High order (p-th): $O(k\mathrm{Comm} k^{1/p} \frac{t^{1+1/p}}{1/p})$

  Randomized product formula, e.g., qDRIFT: $O\left({}^2 t^2/ \right)$:
  (*weak convergence* wrt the diamond norm of Quantum channels)

- LCU, e.g. Truncated Taylor series:

$$O\left(t \frac{\log(t/)}{\log\log(t/)}\right) :$$

- QSP/QSVT: $O\left(t + \frac{\log(1/)}{\log(e+\log(1/)/(t))}\right)$

Helpful References

- Lecture notes on Quantum Algorithms for Scientific Computations by Lin Lin (UC Berkeley) [arXiv:2201.08309]
- Lecture notes on Quantum Algorithms by Andrew Childs (U Maryland)
- A. Gilyen, Y. Su, G.H. Low, N. Wiebe. Quantum singular value transformation and beyond: exponential improvements for quantum matrix arithmetics, [arXiv 1806.01838]

Thank you for your attention!