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

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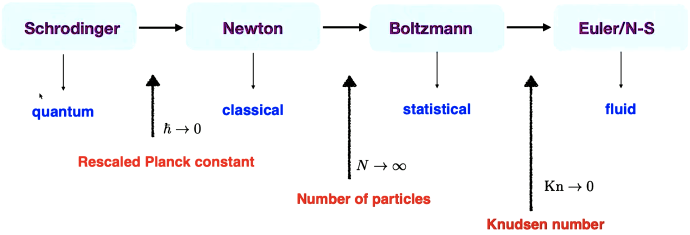
Outline

Part 1: Hamiltonian Simulation (time-independent case)

Different Levels of Physics

multiscale physics fig by Prof. Qin Li

Different Levels of Physics



multiscale physics fig by Prof. Qin Li

Different Levels of Physics

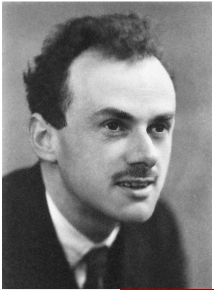
Schrodinger → Newton → Boltzmann → Euler/N-S

quantum | classical | statistical | fluid

$\hbar \to 0$ Rescaled Planck constant

$N \to \infty$ Number of particles

$\mathrm{Kn} \to 0$ Knudsen number



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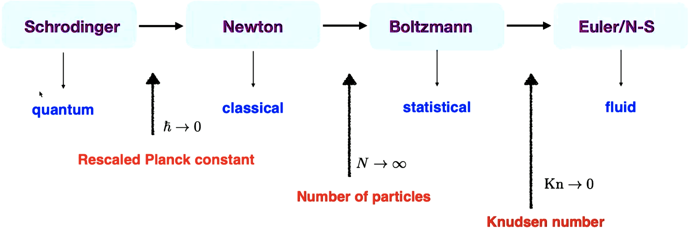

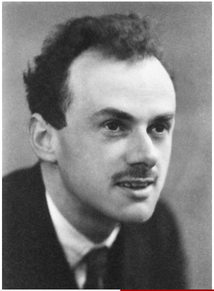

"the underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

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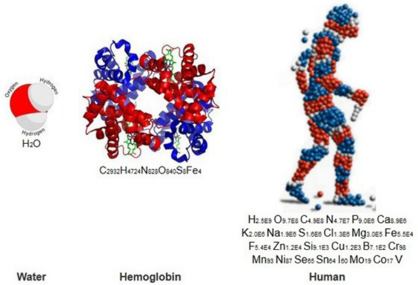
Schrödinger equation for Molecular Dynamics

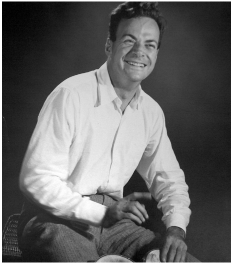


To describe its behaviour: (x: nuclei coordinates, y: electronic coordinates, M: mass of a nucleus, m: mass of an electron.)

$$\hat{H}_{\text{total}} = -\frac{\hbar^2}{2M}\Delta_x - \frac{\hbar^2}{2m}\Delta_y + V(x,y), \quad x \in \mathbb{R}^d, y \in \mathbb{R}^n$$

$$i\hbar\partial_t\psi = \hat{H}_{\text{total}}\psi$$

Quantum Computing 101



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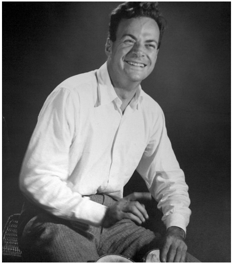

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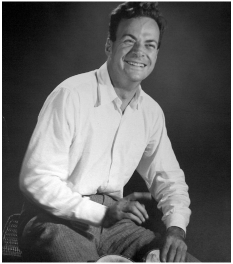

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$$\mathrm{i}\partial_t |\psi(t)\rangle = H(t) |\psi(t)\rangle, \quad |\psi(0)\rangle = |\psi_0\rangle.$$

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

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Examples of H: many-body Hamiltonian

$$H = \sum_{E \in S \subset \{I,X,Y,Z\}^{\otimes n}} \lambda_E E,$$

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

Error Metrics: Specific case v.s. Worst case

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

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

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- Taking into account the **observable**: consider *observable error bounds*. $\|O\| \leq 1$

$$\begin{aligned}
&\left\|\mathcal{U}_{\text{app}}^\dagger O \mathcal{U}_{\text{app}} - e^{iHt} O e^{-\mathrm{i}Ht}\right\| \\
=&\left\|\mathcal{U}_{\text{app}}^\dagger O \mathcal{U}_{\text{app}} - \mathcal{U}_{\text{app}}^\dagger O e^{-\mathrm{i}Ht} + \mathcal{U}_{\text{app}}^\dagger O e^{-\mathrm{i}Ht} - e^{iHt} O e^{-\mathrm{i}Ht}\right\| \\
\leq& 2\left\|\mathcal{U}_{\text{app}} - e^{-\mathrm{i}Ht}\right\| \leq \epsilon.
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- Taking into account **both** and consider *observable expectation* $\left|\left\langle\psi_0\right|\mathcal{U}_{\text{app}}^{\dagger}O\mathcal{U}_{\text{app}}\left|\psi_0\right\rangle - \left\langle\psi_0\right|e^{iHt}Oe^{-\mathrm{i}Ht}\left|\psi_0\right\rangle\right|$

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Specific case v.s. Worst case: Take-away

"Spectrum" of various error measurements:

$$\boxed{\begin{array}{c}\text{Observable}\\\text{expectation}\end{array}} \ll \begin{array}{c}\boxed{\text{Vector norm}}\\\boxed{\text{Observable error bounds}}\end{array} \ll \boxed{\text{Operator norm}}$$

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Specific case v.s. **Worst case**
Taking into account the specific 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.

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Expected Complexity?

2 [Feymann 1985]

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

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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 $H = H_1 + H_2$

$$e^{-\mathrm{i}Ht} \approx \left(e^{-\mathrm{i}H_2 t/L} e^{-\mathrm{i}H_1 t/L}\right)^L$$

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$$e^{-\mathrm{i}Ht} = \left(e^{-\mathrm{i}H_2 t/L} e^{-\mathrm{i}H_1 t/L}\right)^L + \mathcal{O}\left(\|[H_1, H_2]\| t^2 / L\right)$$

The number of Trotter steps $L = \mathcal{O}\left(\|[H_1, H_2]\| t^2 / \epsilon\right)$

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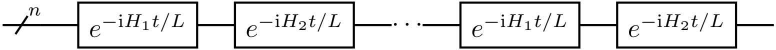

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$$\overset{n}{\not-}\!\!\!-\boxed{e^{-\mathrm{i}H_1 t/L}}-\boxed{e^{-\mathrm{i}H_2 t/L}}-\cdots-\boxed{e^{-\mathrm{i}H_1 t/L}}-\boxed{e^{-\mathrm{i}H_2 t/L}}-$$

$\Rightarrow \mathcal{O}\left(\|[H_1, H_2]\| t^2/\epsilon\right)$ queries to $e^{-\mathrm{i}H_1 s}$ and $e^{-\mathrm{i}H_2 s}$.

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

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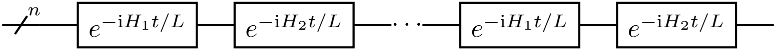

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  - Everything is unitary! No ancilla needed.
  - But it needs $e^{-\mathrm{i}H_j s}$ efficiently implementable.

[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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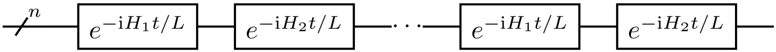

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- Post-Trotter, e.g., truncated Taylor series, quantum signal processing (QSP), quantum singular value transformation (QSVT) [3], etc.

$$e^{-\mathrm{i}Ht} \approx \sum_{k=0}^{K} \frac{(-\mathrm{i}Ht)^k}{k!} = \sum_{k=0}^{K} \sum_{\ell_1,\cdots,\ell_k} \frac{(-\mathrm{i}t)^k}{k!} H_{\ell_1} H_{\ell_2} \cdots H_{\ell_k}.$$

Upshot: $\Rightarrow \mathcal{O}(t \log(t/\epsilon))$

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Upshot: $\Rightarrow \mathcal{O}(t \log(t/\epsilon))$ $\quad\Rightarrow$ Even better, say, $\mathcal{O}(t + \log(1/\epsilon))$?

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Block-Encoding – Definition

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

Idea:

$$U_A = \begin{pmatrix} A & * \\ * & * \end{pmatrix} \quad \rightarrow \text{ancilla qubits}$$

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Definition (Block-encoding)

U_A is an (α, m, ϵ)-block-encoding of A, if

$$\|A - \alpha \left(\langle 0^m| \otimes I_n\right) U_A \left(|0^m\rangle \otimes I_n\right)\| \le \epsilon,$$

for some $\alpha \ge \|A\|$, $m > 0$ and $\epsilon > 0$. Here α is called the *subnormalization* factor and m is the number of ancilla qubits, and n is the number of system qubits. When $\epsilon = 0$, it is also called an (α, m)-block-encoding.

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for some $\alpha \geq \|A\|$, $m > 0$ and $\epsilon > 0$. Here α is called the *subnormalization* factor and m is the number of ancilla qubits, and n is the number of system qubits. When $\epsilon = 0$, it is also called an (α, m)-block-encoding.

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

Block-Encoding – Definition

Let A be a general $2^n \times 2^n$ matrix. $\|A\| \leq \alpha$

Idea:

$$U_A = \begin{pmatrix} \frac{\tilde{A}}{\alpha} & * \\ * & * \end{pmatrix} \qquad \left\|\tilde{A} - A\right\| \leq \epsilon$$

$\rightarrow m$ ancilla qubits,

Definition (Block-encoding)

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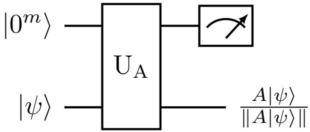
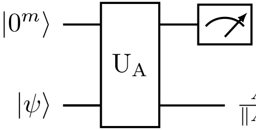


(upon getting 0 in measurement)

Block-Encoding – Definition cont'd



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

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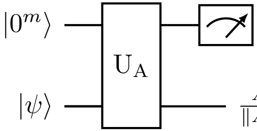

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Question: Well-defined? Not an empty set?

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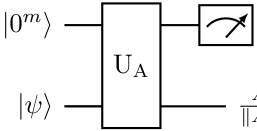

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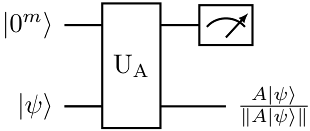

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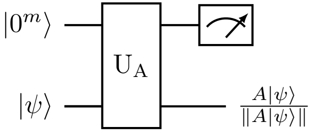

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References: Lecture notes by Lin Lin, QSVT [Gilyen-Su-Low-Wiebe 2018/2019], see also QSP [Low-Chuang 2017], qubitization [Low-Chuang 2016]

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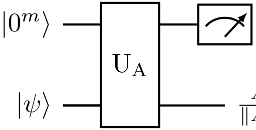

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$$U_A := \begin{pmatrix} W & 0 \\ 0 & I_n \end{pmatrix} \begin{pmatrix} \Sigma & \sqrt{I_n - \Sigma^2} \\ \sqrt{I_n - \Sigma^2} & -\Sigma \end{pmatrix} \begin{pmatrix} V^\dagger & 0 \\ 0 & I_n \end{pmatrix}$$
$$= \begin{pmatrix} A & W\sqrt{I_n - \Sigma^2} \\ \sqrt{I_n - \Sigma^2}V^\dagger & -\Sigma \end{pmatrix}$$

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Sparse Input Model

Question: Efficient to construct?

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Upshot: sparse matrix (Hamiltonian) is ok!

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

$$\begin{aligned} U_{\text{row}} \left|j, s\right\rangle &= \left|j, \text{row}(j,s)\right\rangle, \\ U_{\text{col}} \left|j, s\right\rangle &= \left|j, \text{col}(j,s)\right\rangle, \\ U_{\text{val}} \left|j, k, z\right\rangle &= \left|j, k, z \oplus H_{jk}(t)\right\rangle. \end{aligned} \tag{1}$$

Here $\text{row}(j,s)$ is the row index of the sth nonzero element in the jth column, $\text{col}(j,s)$ is the column index of the sth nonzero element in the jth row.

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

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

Block-Encoding – Properties

Properties: Let U_A be an (α, a, ϵ)-BE of A; U_B be a (β, b, δ)-BE of B

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$$\left\| AB - \alpha\beta(\langle 0|^{\otimes a+b} \otimes I)(I_b \otimes U_A)(I_a \otimes U_B)(|0\rangle^{\otimes a+b} \otimes I) \right\|$$
$$= \left\| AB - \underbrace{\alpha(\langle 0|^{\otimes a} \otimes I)U_A(|0\rangle^{\otimes a} \otimes I)}_{\tilde{A}} \underbrace{\beta(\langle 0|^{\otimes b} \otimes I)U_B(|0\rangle^{\otimes b} \otimes I)}_{\tilde{B}} \right\|$$

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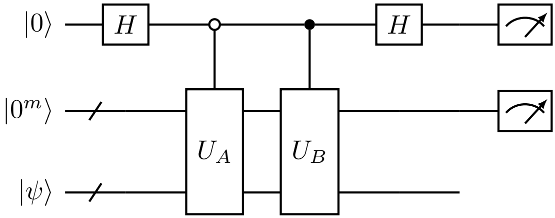
   The following circuit constructs a $(2, m, \delta+\epsilon)$-BE of $A+B$.



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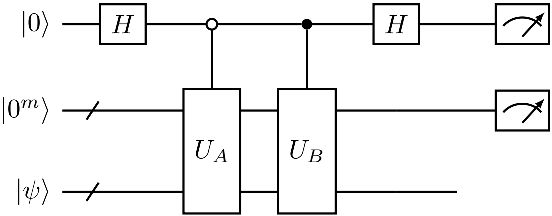

More generally, linear combination of block-encodings can be constructed via Linear Combination of Unitaries (LCU) Lemma.

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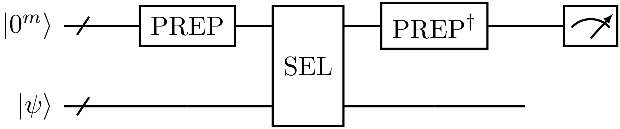
One can get a $(\|c\|_1, \lceil \log_2 L \rceil)$-block-encoding by:

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



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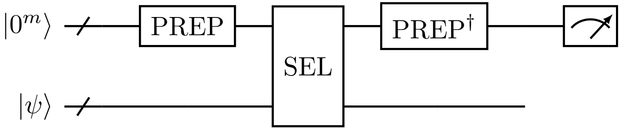

General LCBE: $\max_j m_j + \lceil \log_2 L \rceil$ ancillas

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Matrix Function and Truncated Taylor series

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Number of time steps $L = t/\Delta t = \mathcal{O}(\alpha t)$; $K = \mathcal{O}(\frac{\log(t/\epsilon)}{\log\log(t/\epsilon)})$

$\Rightarrow$ Query Complexity: $\mathcal{O}(\alpha t \frac{\log(t/\epsilon)}{\log\log(t/\epsilon)})$.

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Question: Can we do better?

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

QSVT

$A = W\Sigma V^\dagger \quad f^\diamond(A) := W f(\Sigma) V^\dagger$ Generalized Matrix Function

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Theorem (QSVT with odd real polynomial)

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

$$|P_{\Re}(x)| \leqslant 1, \forall x \in [-1, 1].$$

We can find a sequence of phase factors $\Phi \in \mathbb{R}^{d+1}$ and construct a $(1, m+1)$-block-encoding of $P^\diamond_{\Re}(A)$ that uses $U_A, U_A^\dagger$, m-qubit controlled NOT, and single qubit rotation gates for $\mathcal{O}(d)$ times.

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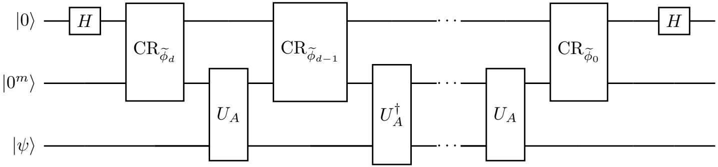

QSVT (Hermitian matrix + arbitary parity)

Theorem (QSVT for Polynomial eigenvalue transformation)
Let U_A be a (α, m, ϵ)-block-encoding of a Hermitian matrix $A \in \mathbb{C}^{2^n \times 2^n}$. Given a d-degree polynomial $P_{\Re}(x) \in \mathbb{R}[x]$ satisfying

$$|P_{\Re}(x)| \leqslant 1/2, \forall x \in [-1, 1].$$

Then for $\delta \geq 0$, there is a quantum circuit that constructs a $(1, m+2, 4d\sqrt{\epsilon/\alpha} + \delta)$-block-encoding of $P_{\Re}^{\diamond}(A/\alpha)$ that uses a single application of controlled-U_A, and d applications of $U_A, U_A^{\dagger}$, and $\mathcal{O}((m+1)d)$ other one- and two-qubit gates.

Optimal Hamiltonian Simulation by QSVT

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

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

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

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

$J_\nu(t)$ denotes Bessel functions of the first kind.

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- $e^{iHt} = e^{i\frac{H}{\alpha}\alpha t}$. WLOG, assume $\alpha = 1$. $e^{itx} = \cos(tx) + i\sin(tx)$
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$$\cos(tx) = J_0(t) + 2\sum_{k=1}^{\infty}(-1)^k J_{2k}(t)T_{2k}(x),$$

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

- This series converges rapidly. Truncating it with

$$r = \Theta\left(t + \frac{\log(1/\epsilon)}{\log(e + \log(1/\epsilon)/t)}\right)$$

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

Optimal Hamiltonian Simulation by QSVT

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

- $e^{iHt} = e^{i\frac{H}{\alpha}\alpha t}$. WLOG, assume $\alpha = 1$. $e^{itx} = \cos(tx) + i\sin(tx)$

Query Complexity: ($\alpha \geq \|H\|$.)

$$\mathcal{O}\left(\alpha t + \frac{\log(1/\epsilon)}{\log(e + \log(1/\epsilon)/(\alpha t))}\right).$$

Optimal Hamiltonian Simulation by QSVT cont'd

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

- 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

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

- 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 $(1, m+2, \epsilon/6)$ of $e^{itH}/2$.

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

Optimal Hamiltonian Simulation by QSVT cont'd

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- Last step: We want to turn $e^{itH}/2$ to e^{itH}.

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Optimal Hamiltonian Simulation by QSVT cont'd

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- Last step: We want to turn $e^{itH}/2$ to e^{itH}. Notice this can be done by QSVT with $P(x) = 3x - 4x^3$.

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

Optimal Hamiltonian Simulation by QSVT cont'd

Given U_H: an $(\alpha, m, 0)$-block-encoding of H.
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- Last step: We want to turn $e^{itH}/2$ to e^{itH}. Notice this can be done by QSVT with $P(x) = 3x - 4x^3$.

  Oblivious Amplitude Amplification (OAA) [4]

  Given a block-encoding U_A of A (and A is close to unitary): $A = \alpha(\langle 0|_m \otimes I_n)U_A(|0\rangle_s \otimes I_n)$. Define $R := I_m - 2\,|0\rangle_m \langle 0|_m$ and

$$W = -U_A(R \otimes I_n)U_A^\dagger(R \otimes I_n)U_A.$$

$$(\langle 0|_m \otimes I_n)W(|0\rangle_m \otimes I_n) = \frac{3}{\alpha}A - \frac{4}{\alpha^3}AA^\dagger A \approx (\frac{3}{\alpha} - \frac{4}{\alpha^3})A.$$

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

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

$$e^{-\mathrm{i}Ht} = \left(e^{-\mathrm{i}H_1 t/L} e^{-\mathrm{i}H_2 t/L}\right)^L + \mathcal{O}(\|[H_1, H_2]\| t^2/L)$$

  High order (p-th): $\mathcal{O}(\|\text{Comm}\|^{1/p} \frac{t^{1+1/p}}{\epsilon^{1/p}})$
  Randomized product formula, e.g., qDRIFT: $\mathcal{O}\left(\alpha^2 t^2/\epsilon\right)$.
  (*weak convergence* wrt the diamond norm of Quantum channels)

- LCU, e.g. Truncated Taylor series:

$$\mathcal{O}\left(\alpha t \frac{\log(t/\epsilon)}{\log\log(t/\epsilon)}\right).$$

- QSP/QSVT: $\mathcal{O}(\alpha t + \frac{\log(1/\epsilon)}{\log(e + \log(1/\epsilon)/(\alpha t))})$

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!