Linear combination of Hamiltonian simulation for non-unitary dynamics with optimal state preparation cost

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Joint work with

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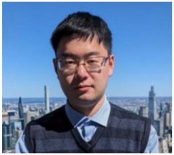

Jin-Peng Liu
(Simons quantum fellow
-> Tsinghua)

An, Liu, **Lin**. Linear combination of Hamiltonian simulation for nonunitary dynamics with optimal state preparation cost. *Phys. Rev. Lett.* 131, 150603 (2023)

An, Childs, **Lin**. Quantum algorithm for linear non-unitary dynamics with near-optimal dependence on all parameters. *arXiv:2312.03916*

Outline

Linear combination of Hamiltonian simulation (LCHS)

Improved LCHS and near-optimal dependence on all parameters

Summary

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Improved LCHS and near-optimal dependence on all parameters

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Time-dependent linear differential equations

$$\frac{du(t)}{dt} = -A(t)u(t), \quad A(t) \in \mathbb{C}^{N\times N},$$
$$u(0) = |u_0\rangle .$$

- $A(t)$ is a general time-dependent matrix.
  If $A(t) = iH(t)$: Hamiltonian simulation.

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- For general $A(t)$, quantum ODE solver approximately implements $\mathcal{T} e^{-\int_0^t A(s)ds}$ (or e^{-At} when $A(s) \equiv A$)

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- For general $A(t)$, quantum ODE solver approximately implements $\mathcal{T} e^{-\int_0^t A(s)ds}$ (or e^{-At} when $A(s) \equiv A$)
- Application: Classical linear ODEs and PDEs, imaginary time quantum evolution, non-Hermitian quantum physics...
- Can generalize to inhomogeneous case e.g., by Duhamel's principle (variation of constants)

Setup

$$\frac{du(t)}{dt} = -A(t)u(t), \quad A(t) \in \mathbb{C}^{N\times N},$$
$$u(0) = |u_0\rangle .$$

- Cartesian decomposition of $A(t)$

$$A(t) = L(t) + iH(t), \quad L(t) = \frac{A(t) + A(t)^\dagger}{2}, \quad H(t) = \frac{A(t) - A(t)^\dagger}{2i}$$

- Assume $L(t) \succeq 0$ for stability

Linear combination of Hamiltonian simulation

Non-unitary evolution operator written as
a Linear Combination of Hamiltonian Simulation problems[1].

Theorem (LCHS)

Suppose $A(t) = L(t) + iH(t)$ *and* $L(t) \succeq 0$, *then*

$$\mathcal{T} e^{-\int_0^t A(s)ds} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} U_k(t) dk.$$

Here $U_k(t)$ *are unitaries that solve the Schrödinger equation*

$$\frac{dU_k(t)}{dt} = -i(kL(t) + H(t))U_k(t), \quad U(0) = I.$$

[1] [An, Liu, **Lin**. Phys. Rev. Lett. (2023); 2303.01029]

Special cases

$$e^{-At} = e^{-(L+iH)t} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} e^{-i(kL+H)t} dk.$$

Non-trivial proof

Only H (the anti-Hermitian part)

$$e^{-iHt} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} e^{-iHt} dk$$

Proof: $\frac{1}{\pi(1+k^2)}$ is the Cauchy probability distribution function

+

Only L (the Hermitian part)

$$e^{-Lt} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} e^{-ikLt} dk$$

Proof: the Fourier transform of $\frac{1}{\pi(1+k^2)}$ is $e^{-|x|}$

Special cases used in [Zeng, Sun, and Yuan. 2109.15304; Huo, and Li, 2109.07807]

Algorithms

LCHS identity + integral truncation ($K = \mathcal{O}(1/\epsilon)$) + quadrature

$$\mathcal{T} e^{-\int_0^t A(s)ds} \approx \int_{-K}^{K} \frac{1}{\pi(1+k^2)} U_k(t) dk \approx \sum_j c_j U_{k_j}(t).$$

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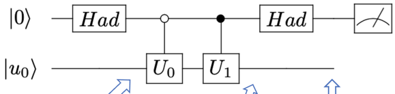
Flexible implementation:

- For $U_{k_j}(t)$: any Hamiltonian simulation algorithm
- Linear combination:
  - Fully quantum: linear combination of unitaries (LCU) technique[1]
  - Hybrid quantum classical: Importance sampling[2,3,4]

[1] [Childs, and Wiebe. Quantum Inf. Comput. (2012)]
[2] [Lin, and Tong. PRX Quantum (2022)]
[3] [Wan, Berta, and Campbell. Phys. Rev. Lett. (2022)]
[4] [Wang, McArdle, and Berta. arXiv:2302.01873 (2023)]

Quantum implementation: LCU

A toy example: computing $\frac{1}{2}(U_0 + U_1)\,|u_0\rangle$



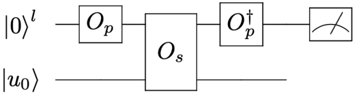
$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\,|u_0\rangle$$

$$\frac{1}{\sqrt{2}}(|0\rangle\, U_0\, |u_0\rangle + |1\rangle\, U_1\, |u_0\rangle)$$

$$\frac{1}{2}\,|0\rangle\,(U_0 + U_1)\,|u_0\rangle + \frac{1}{2}\,|1\rangle\,(U_0 - U_1)\,|u_0\rangle)$$

$$Had = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \begin{cases} |0\rangle & \to \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ |1\rangle & \to \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \end{cases}$$

General: computing $\sum_j c_j U_{k_j}(t)$



Prepare Oracle $O_p : |0\rangle \to \frac{1}{\sqrt{\|c\|_1}} \sum_j \sqrt{c_j}\,|j\rangle$

Select Oracle $O_s = \sum_j |j\rangle\langle j| \otimes U_{k_j}(t)$

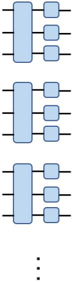
Hybrid implementation: Importance sampling

$$u(t) \approx \sum_j c_j U_{k_j}(t) |u_0\rangle \implies u(t)^* O u(t) \approx \sum_{j,j'} c_j^* c_{j'} \langle u_0 | U_{k_j}^\dagger (t) O U_{k_{j'}}(t) | u_0 \rangle$$

Classical

Sample (j, j') with probability $\propto |c_j^* c_{j'}|$ ⇒

Quantum



$o_1 = \langle u_0 | U_{k_{j_1}}^\dagger (t) O U_{k_{j_1'}}(t) | u_0 \rangle$

$o_2 = \langle u_0 | U_{k_{j_2}}^\dagger (t) O U_{k_{j_2'}}(t) | u_0 \rangle$

$o_3 = \langle u_0 | U_{k_{j_3}}^\dagger (t) O U_{k_{j_3'}}(t) | u_0 \rangle$

⋮

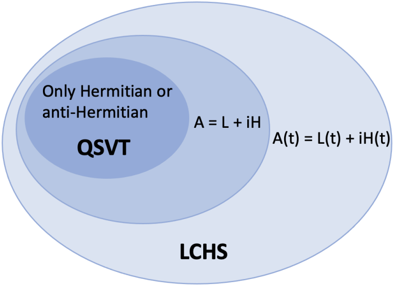
Classical

⇒ Average all the o's

Comparison with QSVT

Solving (time-independent) differential equations is an eigenvalue transformation instead of singular value transformation problem.

LCHS vs Quantum singular value transformation (QSVT)



QSVT: Gilyen, Su, Low, Wiebe, 1806.01838

Previous works on general linear differential equations

- (Berry, 1010.2745), Linear system approach.
- (Berry, Childs, Ostrander, Wang, 1701.03684), time-independent, truncated Taylor series, linear system.
- (Childs, Liu, 1901.00961), Spectral method, linear system.
- (Berry, Costa, 2212.03544) Truncated Dyson, linear system.
- (Fang, Lin, Tong, 2208.06941) Time marching.
- (Jin, Liu, Yu, 2212.13969) Schrödingerization.

See Di Fang's tutorial talk on *Quantum algorithms for dynamics simulation*, IPAM Program Mathematical and Computational Challenges in Quantum Computing, Fall 2023

Comparison with linear system approach

LCHS vs other quantum ODE algorithms

Hamiltonian simulation

Schrödinger equation

$$U_{M-1} \cdots U_2 U_1 U_0 \left| u_{\mathrm{in}} \right\rangle$$

Single input state

ODE algorithms

$$\frac{du}{dt} = -Au + b$$

discretization

$$\frac{u(t+h)-u(t)}{h} \approx -Au(t) + b$$

$$\begin{pmatrix} I & & & & \\ -(I-hA) & I & & & \\ & -(I-hA) & I & & \\ & & \ddots & \ddots & \\ & & & -(I-hA) & I \end{pmatrix} \begin{pmatrix} u(0) \\ u(h) \\ u(2h) \\ \vdots \\ u(T) \end{pmatrix} = \begin{pmatrix} u_0 \\ b \\ b \\ \vdots \\ b \end{pmatrix}$$

Require multiple copies of RHS

Apply HHL algorithm (or more advanced ones)

Comparison

Method	Query complexity	
	A	u_0
Dyson [1]	$\widetilde{\mathcal{O}}\left(q\alpha T\log^2\left(\frac{1}{\epsilon}\right)\right)$	$\mathcal{O}\left(q\alpha T\log\left(\frac{1}{\epsilon}\right)\right)$
LCHS	$\widetilde{\mathcal{O}}\left(q^2\alpha T/\epsilon\right)$	$\mathcal{O}(q)$

Table: Comparison between LCHS and the best linear system approach. Here $\alpha = \max_t \|A(t)\|$, $q = \|u_0\|/\|u(T)\|$.

- LCHS achieves optimal state preparation cost: lower bound is $\Omega(q)$.
- LCHS is a first order method (query to A scales as $\mathcal{O}(1/\varepsilon)$).

[1] Berry-Costa, arXiv:2212.03544 (2022)

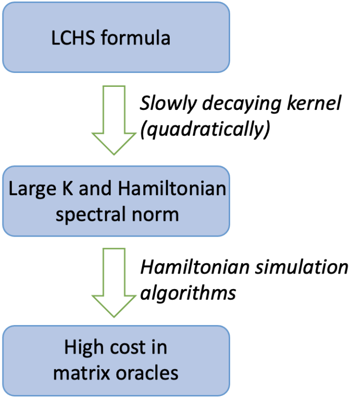
Drawback

$$\mathcal{T}e^{-\int_0^t A(s)ds} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} U_k(t)dk.$$

$$\frac{dU_k(t)}{dt} = -i(kL(t)+H(t))U_k(t), \quad U(0) = I.$$

- Main drawback: only first-order convergence ($K = \mathcal{O}(1/\epsilon)$)
- Improved LCHS: better kernel function

$$\frac{1}{\pi(1+k^2)} \quad \rightarrow \quad \frac{f(k)}{1-ik}$$



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Why possible?

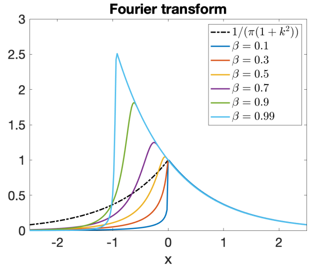
Change kernel:

$$e^{-(L+iH)t} = \int_{\mathbb{R}} \frac{f(k)}{1-ik} e^{-i(kL+H)t} dk$$

Only need $L \succeq 0$. Scalar case with $H = 0$,

$$e^{-x} = \int_{\mathbb{R}} \frac{f(k)}{1-ik} e^{-ikx} dk, \quad x \geq 0.$$

- The same Fourier transform on the positive real axis
- Flexibility on the negative real axis



Theorem (Improved LCHS)

Suppose $A(t) = L(t) + iH(t)$ and $L(t) \succeq 0$, then

$$\mathcal{T} e^{-\int_0^t A(s)ds} = \int_{\mathbb{R}} \frac{f(k)}{1-ik} U_k(t) dk.$$

Here $U_k(t)$ are unitaries that solve the Schrödinger equation

$$\frac{dU_k(t)}{dt} = -i(kL(t) + H(t))U_k(t), \quad U(0) = I,$$

and $f(z)$ is a function of $z \in \mathbb{C}$, such that

1. *(Analyticity) $f(z)$ is analytic on the lower half plane $\{z : \text{Im}(z) < 0\}$ and continuous on $\{z : \text{Im}(z) \leq 0\}$,*
2. *(Decay) there exist $\alpha > 0, C > 0$ such that $|z|^\alpha |f(z)| \leq C$ when $\text{Im}(z) \leq 0$,*
3. *(Normalization) $\int_{\mathbb{R}} \frac{f(k)}{1-ik} dk = 1$.*

[An, Childs, **Lin**. 2312.03916]

Kernel functions

$$\mathcal{T}e^{-\int_0^t A(s)ds} = \int_{\mathbb{R}} \frac{f(k)}{1-ik} U_k(t)dk.$$

- Original LCHS:

$$f(z) = \frac{1}{\pi(1+iz)}$$

- Improved LCHS with near exponential decay $e^{-c|z|^\beta}$

$$f(z) = \frac{1}{C_\beta e^{(1+iz)^\beta}}, \quad \beta \in (0,1)$$

- The asymptotic decay rate is near optimal (cannot reach $e^{-c|z|}$).

Complexity

Method	Query complexity	
	$A(t)$	u_0
Dyson[1]	$\widetilde{\mathcal{O}}\left(q\alpha T\left(\log\left(\frac{1}{\epsilon}\right)\right)^2\right)$	$\mathcal{O}\left(q\alpha T\log\left(\frac{1}{\epsilon}\right)\right)$
Time-marching[2]	$\widetilde{\mathcal{O}}\left(q\alpha^2 T^2\log\left(\frac{1}{\epsilon}\right)\right)$	$\mathcal{O}\left(q\right)$
Original LCHS	$\widetilde{\mathcal{O}}\left(q^2\alpha T/\epsilon\right)$	$\mathcal{O}(q)$
Improved LCHS	$\widetilde{\mathcal{O}}\left(q\alpha T\left(\log\left(\frac{1}{\epsilon}\right)\right)^{1+1/\beta}\right)$	$\mathcal{O}(q)$

Table: Here $\alpha = \max_t \|A(t)\|$, $q = \|u_0\|/\|u(T)\|$, and $0 < \beta < 1$.

Optimal state preparation cost and near-optimal matrix complexity at the same time!

[1][Berry, and Costa. arXiv:2212.03544 (2022)]
[2][Fang, Lin, and Tong. Quantum (2023)]

Proof of the LCHS formula

$$O_L(t) := e^{-(L+iH)t} = \int_{\mathbb{R}} \frac{f(k)}{1-ik} e^{-i(kL+H)t} dk =: O_R(t).$$

Idea: to show that O_L and O_R satisfy the same ODE

$$\frac{dO_L}{dt} = -(L+iH)O_L(t),$$
$$\frac{dO_R}{dt} = -(L+iH)O_R(t) + \mathcal{P}\int_{\mathbb{R}} f(k) e^{-i(kL+H)t} dk.$$

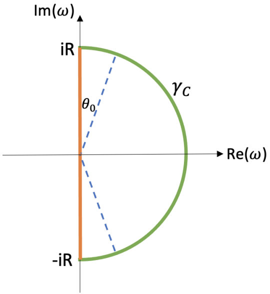
It suffices to show:

$$\mathcal{P}\int_{\mathbb{R}} f(k) e^{-i(kL+H)t} dk = 0.$$

We use Cauchy's integral theorem.

Proof of the LCHS formula

$$\int_{-R}^{R} f(k)e^{-i(kL+H)t}dk$$
$$= -i\int_{-iR}^{iR} f(-i\omega)e^{-\omega Lt-iHt}d\omega$$
$$= -i\int_{\gamma_C} f(-i\omega)e^{-\omega Lt-iHt}d\omega$$
$$= -i\left(\int_{-\frac{\pi}{2}}^{-\frac{\pi}{2}+\theta_0} + \int_{\frac{\pi}{2}-\theta_0}^{\frac{\pi}{2}} + \int_{-\frac{\pi}{2}+\theta_0}^{\frac{\pi}{2}-\theta_0}\right)\cdots d\theta$$



Suppose $L \succ 0$ and choose proper θ_0, then all the integrals vanish as $R \to \infty$, so we prove the LCHS formula for $L \succ 0$.

Take the limit to prove for $L \succeq 0$.

Optimality of the kernel function

Theorem (Optimality)

Suppose $f(z)$ is a function of $z \in \mathbb{C}$, such that

1. *(Analyticity) $f(z)$ is analytic on the lower half plane $\{z : \mathrm{Im}(z) < 0\}$ and continuous on $\{z : \mathrm{Im}(z) \leq 0\}$,*
2. *(Boundedness) $|f(z)| \leq \widetilde{C}$ on $\{z : \mathrm{Im}(z) \leq 0\}$,*
3. *(Exponential decay) for any $z = k \in \mathbb{R}$, we have $|f(k)| \leq \widetilde{c}e^{-c|k|}$.*

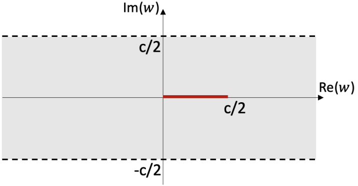
Then $f(z) = 0$ for all $z \in \{z : \mathrm{Im}(z) \leq 0\}$ (including all $z \in \mathbb{R}$).

Proof techniques: Phragmén–Lindelöf principle (generalization of maximum modulus principle)

Optimality of the kernel function

Sketch of the proof:

1. Exponential decay on the real axis $\Longrightarrow$ Exponential decay on the entire lower half plane (by the Phragmén–Lindelöf principle)
2. Consider the extended Fourier transform on $w \in \{-c/2 < \text{Im}(w) < c/2\}$,
$$F(w) = \int_{\mathbb{R}} f(k) e^{-iwk} dk.$$
3. Prove that $F(w)$ is analytic and $F(w) = 0$ on $w \in (0, c/2) \Longrightarrow F(w) \equiv 0$ (by the identity theorem) and thus $f(k) = 0$ on real axis.
4. $f(z) \equiv 0$ for all z.



Outline

Conclusion

- Any linear non-unitary dynamics can be represented as a linear combination of unitary problems.
- LCHS can be implemented quantumly or in a hybrid fashion.
- The quantum improved LCHS algorithm is near-optimal for general ODEs.
- Complexity improvement for time-independent problems and Gibbs state preparation.

Future work - direct extension

- Even better complexity via
  - Better Hamiltonian simulation
  - Better numerical quadrature: (Gaussian: $K = \mathcal{O}((\log(1/\epsilon))^{1/\beta})$)

$$\min \max_j |k_j| \quad \text{s.t.} \quad \int_{\mathbb{R}} \frac{f(k)}{1 - ik} U_k(t) dk \approx \sum_j c_j U_{k_j}(t)$$

- Nonlinear non-unitary dynamics? General matrix functions?
- Different stability condition?

Acknowledgment

Thank you for your attention!

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https://math.berkeley.edu/~linlin/