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

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(joint work with Jin-Peng Liu, Lin Lin)
(arXiv:2303.01029)

Oct 5, 2023

Hamiltonian simulation

$$i\frac{d}{dt}u(t) = H(t)u(t), \quad 0 \leq t \leq T, \quad H \text{ is Hermitian}$$

- Hamiltonian simulation algorithms: Trotter methods, Quantum walk, Truncated Taylor/Dyson series, Quantum single processing (QSP), Qubitization, Quantum singular value transformation (QSVT), Randomization methods, etc

Beyond Hamiltonian simulation

- In this talk, we focus on non-unitary dynamics beyond Hamiltonian simulation problem.
- Why do we care about non-unitary dynamics?

Differential equations

Differential equations are ubiquitous in various fields of science and engineering

- Physics: the motion of particles, the flow of fluids, and the propagation of waves
- Chemistry: chemical reactions, chemical thermodynamics
- Biology: the spread of diseases, the growth of populations
- Economics: stocks, bonds, options, economic growth
- ......

High-dimensional in practice, significant challenges in classical scientific computing

Open quantum dynamics

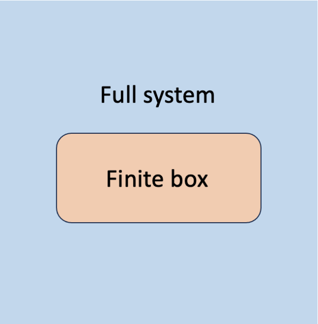
- Many problems in quantum dynamics are defined in an infinite space: computationally intractable
  - molecular scattering, photodissociation, nanotransport...
- Complex absorbing potential method[1]: using effective Hamiltonian with correction terms on a finite-sized box

$$\Longrightarrow \text{“non-Hermitian Hamiltonian”}$$

$$i\partial_t u(\mathbf{r},t) = \Big(\underbrace{-\frac{1}{2}\Delta_{\mathbf{r}} + V_R(\mathbf{r},t)} - iV_I(\mathbf{r})\Big)\, u(\mathbf{r},t).$$

Standard Hamiltonian anti-Hermitian part

Absorbing potential Hermitian part



[1]Vibok-Balint-Kurti, J. Phys. Chem. 96, 8712 (1992)

Convection-diffusion equation

Dynamics of physical systems with the presence of both convection and diffusion processes

$$\frac{\partial u(t,x)}{\partial t} = \Delta_x u(t,x) - \nabla_x \cdot u(t,x) + f(t,x).$$

Diffusion
Hermitian part

Convection
anti-Hermitian part

External source
Inhomogeneous term

Optimization

- Suppose that we would like to minimize an objective function $f(x)$
- Gradient descent:

$$x_{k+1} = x_k - \eta \nabla f(x_k)$$

- Gradient flow:

$$\frac{dx}{dt} = -\nabla f(x)$$

Setup

$$\frac{du(t)}{dt} = -A(t)u(t), \quad u(0) = u_0$$

- $A(t)$ is a general time-dependent matrix and can be decomposed into its Hermitian and anti-Hermitian parts as

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

- Quantum algorithm for this ODE aims at preparing a quantum state encoding the solution in its amplitude:

$$|u(T)\rangle = \frac{1}{\|u(T)\|} \sum_{j=0}^{N-1} u_j(T) |j\rangle .$$

Main result

Any non-unitary dynamics is related to Hamiltonian simulation problems, in the sense that any non-unitary evolution operator can be written as a linear combination of Hamiltonian simulation problems (LCHS).

Theorem

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

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

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 $e^{-|x|}$ is $\frac{1}{\pi(1+k^2)}$

[2] Zeng-Sun-Yuan, arXiv:2109.15304 (2022) Huo-Li, Quantum 7, 916 (2023).

Implementation

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

Flexible implementation:

- For $U_{k_j}(t)$: any Hamiltonian simulation algorithm (*e.g.*, Trotter formula)
- The linear combination step:
  - Quantum: linear combination of unitaries (LCU) technique[3]
  - Hybrid: Importance sampling[4,5,6]

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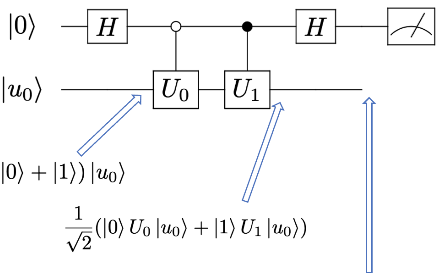
[3]Childs-Wiebe, Quantum Inf. Comput. 12, 901-924 (2012)
[4]Lin-Tong, PRX Quantum 3, 010318 (2022)
[5]Wan-Berta-Campbell, Phys. Rev. Lett. 129, 030503 (2022)
[6]Wang-McArdle-Berta, arXiv:2302.01873 (2023)

Quantum implementation: LCU

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

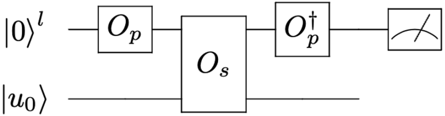


$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\,|u_0\rangle$$

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

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

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



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

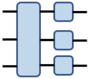
Select Oracle $O_s = \sum_j |j\rangle\langle j| \otimes U_{k_j}(t)$

Hybrid implementation: Importance sampling

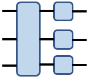
$$u(t) \approx \sum_{j} c_j U_{k_j}(t)\,|u_0\rangle \quad \Longrightarrow \quad \langle u(t)|O|u(t)\rangle \approx \sum_{j,j'} c_j c_{j'} \,\langle u_0|U_{k_j}^{\dagger}(t) O U_{k_{j'}}(t)|u_0\rangle\,.$$

Classical **Quantum** **Classical**

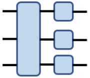
Sample (j, j') with probability $p \propto c_j c_{j'}$



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



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



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

⋮ ⋮

Average all the o's

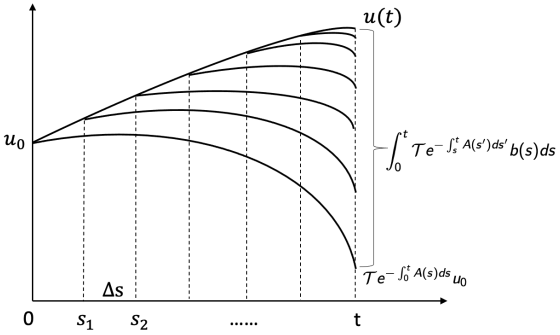
Generalization: inhomogeneous case

$$\frac{du(t)}{dt} = -A(t)u(t) + b(t).$$

$$u(t) = \mathcal{T}e^{-\int_0^t A(s)ds}u(0) + \int_0^t \mathcal{T}e^{-\int_s^t A(s')ds'}b(s).$$

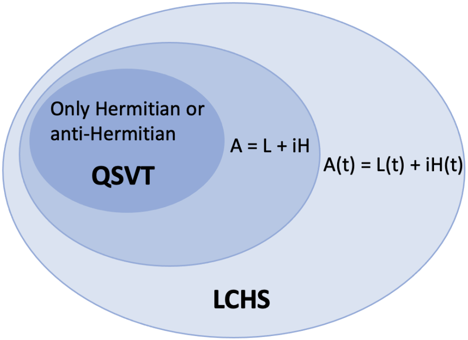
Duhamel's Principle:

- We can view $b(t)$ as a perturbation term of the homogeneous equations without $b(t)$
- The general solution is another linear combination of non-unitary operators $\mathcal{T}e^{-\int_s^t A(s')ds'}$
- Linear combination of LCHS



Comparison

LCHS vs Quantum singular value transformation (QSVT)



Existing quantum algorithms for ODEs

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

1. Time discretization: $\frac{u(t+h)-u(t)}{h} \approx -Au(t) + b$
2. Consider the equations for $[u(0); u(h); u(2h); \cdots]$, then

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

3. Apply quantum linear system algrithms (e.g., HHL)
4. Measurement

Existing quantum algorithms for ODEs

Different strategies:

- Hamiltonian simulation: directly apply numerical integrators to the initial state
- General ODE: transfer to a large linear system problem and apply HHL

High state preparation cost in general ODE algorithms due to the usage of linear system algorithms

- Even optimal linear system algorithm requires $\mathcal{O}(\kappa \log(1/\epsilon))$ state preparation cost, where κ is the condition number of the linear systems and can be large in solving ODEs.
- A lower bound for solving linear systems: $\Omega(\kappa)$ state preparation cost for any matrix and worst-case vector.

Comparison

LCHS vs other quantum ODE algorithms

Hamiltonian simulation

Schrödinger equation

↓

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

↓

Single input state

ODE algorithms

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

↓ discretization

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

Require multiple copies of RHS

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

Apply HHL algorithm (or more advanced ones)

[7] Berry, J. Phys. A 47, 105301 (2014)

Somma-Subaşı, PRX Quantum 2, 010315 (2021)

Comparison

Method	Query complexity	
	A	u_0
Dyson [8]	$\widetilde{\mathcal{O}}\left(\widetilde{q}\alpha T \log^2\left(\frac{1}{\epsilon}\right)\right)$	$\mathcal{O}\left(\widetilde{q}\alpha T \log\left(\frac{1}{\epsilon}\right)\right)$
LCHS	$\widetilde{\mathcal{O}}\left(q^2\alpha T/\epsilon\right)$	$\mathcal{O}(q)$

Table: Comparison between LCHS and the state-of-the-art truncated Dyson series method. Here $\alpha = \max_t \|A(t)\|$, $q = \|u_0\|/\|u(T)\|$ and $\widetilde{q} = \max_t \|u(t)\|/\|u(T)\|$ (we have $q \leq \widetilde{q}$)

- LCHS achieves optimal state preparation cost: lower bound is $\Omega(q)$.

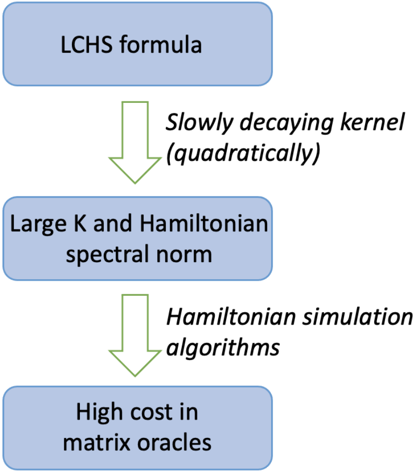
[8] Berry-Costa, arXiv:2212.03544 (2022)

Drawback

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

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

- Main drawback: linear convergence in queries to the matrix
- Solutions:
  - Interaction picture Hamiltonian simulation
  - Better kernel function (ongoing work)



Improved LCHS: interaction picture

$$\frac{du}{dt} = -(L + iH(t))u,$$

- LCHS suggests that the dynamics is the linear combination of $U_k(t)$ where

$$i\frac{dU_k(t)}{dt} = (kL + H(t))U_k(t)$$

- Difficulty: k can be large, and Hamiltonian simulation algorithms typically depend linearly on the Hamiltonian spectral norm.
- Interaction picture[9]: suppose L is fast-forwardable,

$$U_{k,I}(t) = e^{ikLt}U_k(t) \quad \Longrightarrow \quad \frac{dU_{k,I}(t)}{dt} = e^{ikLt}H(t)e^{-ikLt}U_{k,I}(t)$$

- Overall complexity: $\mathcal{O}(q)$ queries to u_0 and $\widetilde{\mathcal{O}}(qT\|H\| \operatorname{poly}\log(1/\epsilon))$ queries to the Hamiltonians

[9] Low-Wiebe, arXiv:1805.00675 (2018)

Summary

- Any linear non-unitary dynamics can be represented as a linear combination of Hamiltonian simulation problems.
- The LCHS method can be implemented coherently or in a hybrid fashion.
- The LCHS method achieves low (and optimal) state preparation cost.
- The drawback of current LCHS method is its $1/\epsilon$ dependence in terms of matrix access, which can be overcome by interaction picture Hamiltonian simulation for fast-forwardable systems, or by a better kernel function (ongoing work).
- A related approach: Schrödingerization by Jin, Liu and Yu [arXiv:2212.13969]

D. An, J. Liu, L. Lin. *Linear combination of Hamiltonian simulation for non-unitary dynamics with optimal state preparation cost*. arXiv:2303.01029 (2023)

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Thank you!