Higher-order quantum transformations of Hamiltonian dynamics

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Presentation slides

arXiv:2303.09788

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Outline

I. Motivation & main results

II. Overview of our algorithm

III. Instance of quantum functional programming

IV. Application

V. General framework of higher-order transformation of Hamiltonian dynamics

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(approximate) Hamiltonian simulation

- Hamiltonian simulation is a possible application of quantum computers

Input:

$$H = \begin{pmatrix} * & \cdots & * \\ \vdots & \ddots & \vdots \\ * & \cdots & * \end{pmatrix}$$

Description of Hamiltonian
(classical)

Output:

$$U \simeq e^{-iHt}$$

Hamiltonian dynamics
(quantum)

- Many algorithms have been proposed (e.g. qDRIFT[1], QSVT based[2])

[1] E. Campbell, PRL **123**, 070503 (2019). [2] Low, Guang Hao, and Isaac L. Chuang, Quantum **3**, 163 (2019).

Problems with Hamiltonian simulation

Problem: Classical description of target Hamiltonian is required in existing methods

$$H_{\mathrm{known}} = \begin{pmatrix} * & \cdots & * \\ \vdots & \ddots & \vdots \\ * & \cdots & * \end{pmatrix} \Rightarrow U \simeq e^{-iH_{\mathrm{known}}t}$$

E.g. qDRIFT, QSVT-based

$$H_{??} \Rightarrow f(H_{??})$$

New methods needed

E.g. negative time-evolution (simulating inverse unitary) $e^{-iHt} \Rightarrow e^{+iHt}$

Our approach

Transformation of Hamiltonian is formulated as:

"Higher-order transformation on Hamiltonian dynamics"

Our approach

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(black-box) quantum operation → quantum operation

Our approach

Transformation of Hamiltonian is formulated as:

"Higher-order transformation on Hamiltonian dynamics"

(black-box) quantum operation → quantum operation

Previous work

$$H_{\text{known}} = \begin{pmatrix} * & \cdots & * \\ \vdots & \ddots & \vdots \\ * & \cdots & * \end{pmatrix}$$

$$e^{-iH_{\text{known}}t}$$

Our work

① e^{-iHt}

?

② Function f

$$H \mapsto f(H)$$

$$e^{-if(H)t}$$

?

Result

deterministic & approximate

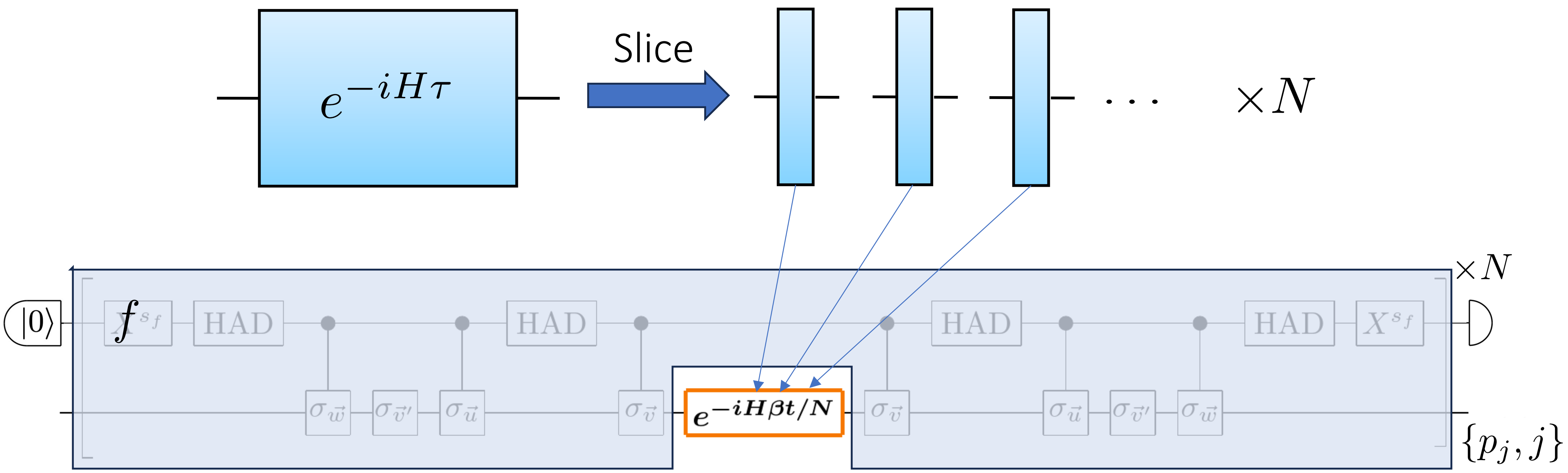
Higher-order transformation $e^{-iHt} \mapsto e^{-if(H)t}$ by linear map f of unknown Hamiltonian

Figure of merit: **Overall runtime**
(Not #queries to dynamics)

Result

Deterministic & Approximate

Higher-order transformation $e^{-iHt} \mapsto e^{-if(H)t}$ by linear map f of unknown Hamiltonian



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Simulation of $e^{-if(H)t}$ (known H)

To get a clue about the higher-order algorithm, we first see how to simulate $e^{-if(H)t}$ for known H

① Decompose $f(H)$ into linear combination of simpler Hamiltonians H_j

$$f(H) = \sum_j h_j H_j$$

② Simulate RHS by qDRIFT

Extendable to unknown H

① Decomposition of f (unknown H)

We can obtain a decomposition of $f(H)$ with H-independent parameters using Pauli transfer matrix (PTM) of f

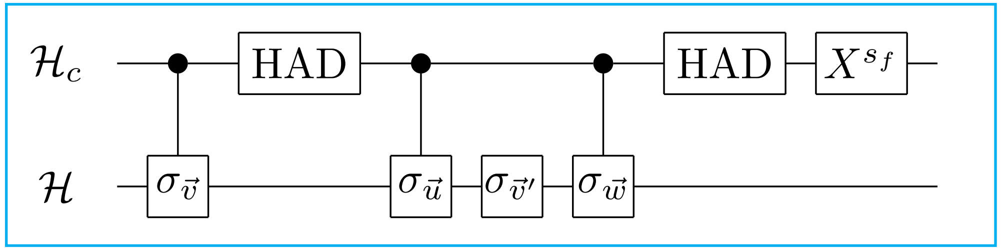
H -independent

$$\begin{pmatrix} f(H) & 0 \\ 0 & -f(H) \end{pmatrix} = \sum_j \boxed{p_j V_{f,j}} \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \boxed{V_{f,j}^{\dagger}}$$

Designed using functional programming

p_j : Defined using PTM of f

$V_{f,j} :=$



Pauli transfer matrix (PTM)

We describe n-qubit case:

$$H = \sum_{\vec{u}} c_{\vec{u}} \sigma_{\vec{u}} \Leftrightarrow \begin{pmatrix} 0 \\ c_{(0,\ldots,1)} \\ \vdots \\ c_{(3,\ldots,3)} \end{pmatrix} \in \mathbb{R}^{4^n}$$

$$\sigma_{\vec{v}} := \sigma_{v_1} \otimes \cdots \otimes \sigma_{v_n}$$

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$\Rightarrow$

Hermitian preserving linear map f

$$\text{s.t. } f(\sigma_{\vec{u}}) = \sum_{\vec{w}} \gamma_{\vec{w},\vec{u}} \sigma_{\vec{w}} \Leftrightarrow$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \gamma_{(0,\dots,1),(0,\dots,1)} & \cdots & \gamma_{(0,\dots,1),(3,\dots,3)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \gamma_{(3,\dots,3),(0,\dots,1)} & \cdots & \gamma_{(3,\dots,3),(3,\dots,3)} \end{pmatrix}$$

PTM of "physically realizable linear map"

Pauli transfer matrix (PTM)

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$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \gamma_{(0,\ldots,1),(0,\ldots,1)} & \cdots & \gamma_{(0,\ldots,1),(3,\ldots,3)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \gamma_{(3,\ldots,3),(0,\ldots,1)} & \cdots & \gamma_{(3,\ldots,3),(3,\ldots,3)} \end{pmatrix}$$

PTM of "physically realizable linear map"

$$p_j := \frac{2|\gamma_{\vec{w},\vec{u}}|}{16^n \beta} \propto |\gamma_{\vec{w},\vec{u}}|$$

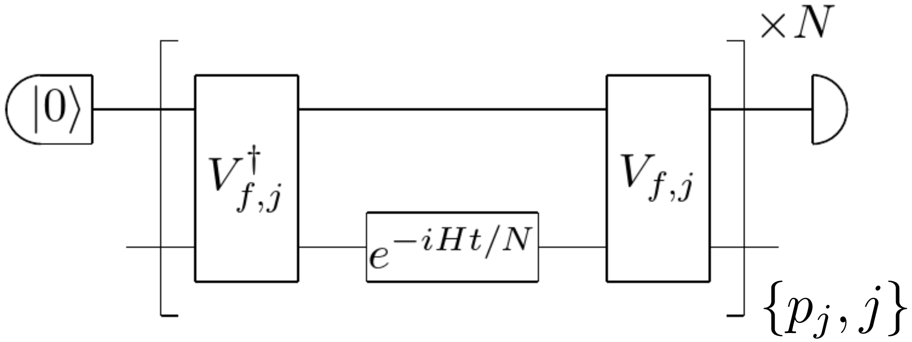
② Simulation of $f(H)$ (unknown H)

Decomposition of $f(H)$ can be used to implement $e^{-if(H)t}$ for unknown H

$$\begin{pmatrix} f(H) & 0 \\ 0 & -f(H) \end{pmatrix} = \sum_j p_j V_{f,j} \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} V_{f,j}^\dagger$$

Hamiltonian simulation with random sampling

$$e^{-if(H)t} \simeq$$



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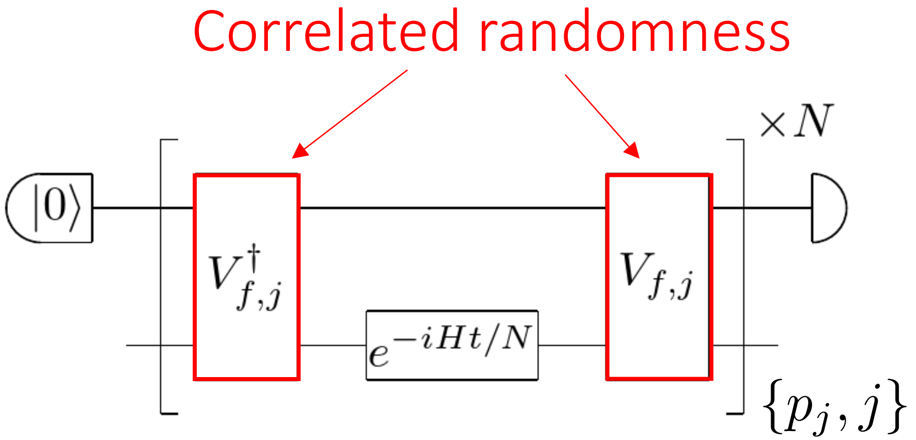


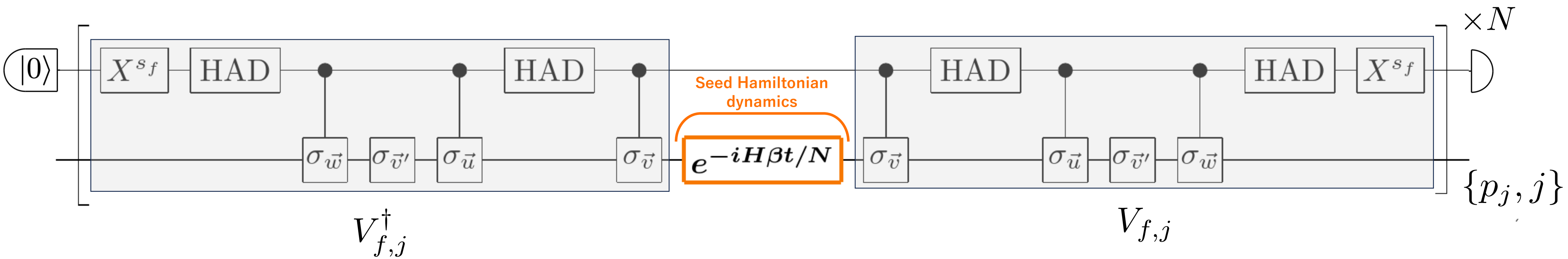
Our algorithm

We developed an algorithm applicable to arbitrary physically realizable linear map f.

Runtime: $O(\beta^2 t^2 n/\epsilon)$

$\beta :=$ (Function of PTM), ϵ : allowed error

$$\boxed{e^{-if(H)t}} \simeq$$



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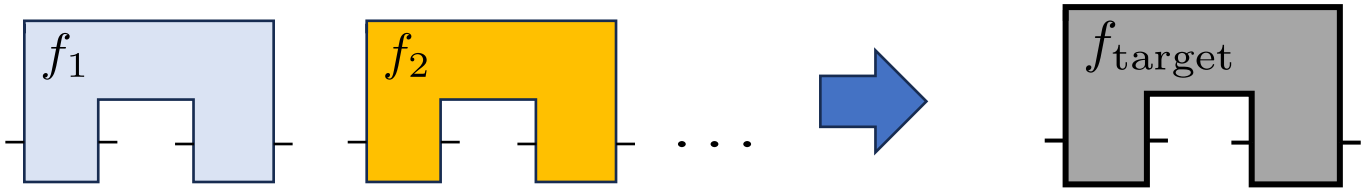
Quantum functional programming

Quantum functional programming:



E.g. concatenating higher-order transformations

Our algorithm: construct subroutine by concatenating seven functions

$$(\text{Subroutine function}) = g^{(7)}_{f,\vec{w},\vec{u}} \circ g^{(6)} \circ g^{(5)}_{\vec{w}} \circ g^{(4)} \circ g^{(3)}_{\vec{u}} \circ g^{(2)} \circ g^{(1)}$$

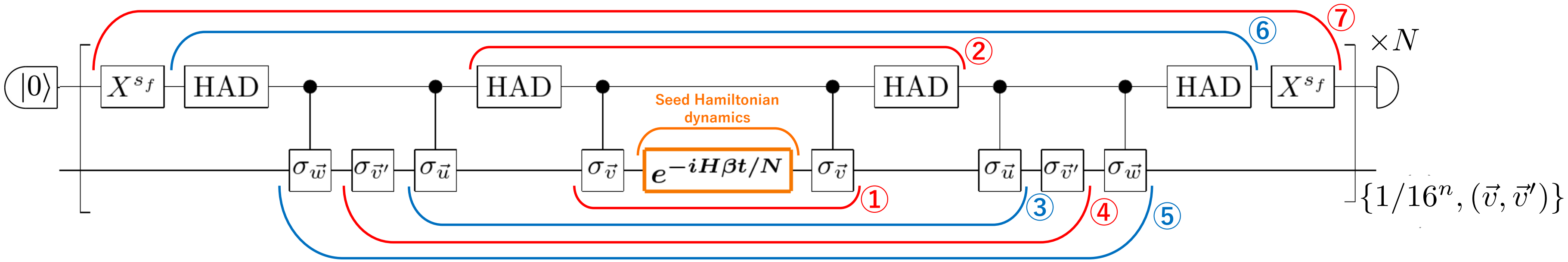
$V_{f,j}$ is naturally derived from this construction

Detail of functional programming instance

$$I \otimes H = \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \xrightarrow{\textcircled{1}} \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} \xrightarrow{\textcircled{2}} \begin{pmatrix} H & H \\ H & H \end{pmatrix} \xrightarrow{\textcircled{3}} \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix}$$

$$\xrightarrow{\textcircled{4}} c_{\vec{u}} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \xrightarrow{\textcircled{5}} c_{\vec{u}} \begin{pmatrix} 0 & \sigma_{\vec{w}} \\ \sigma_{\vec{w}} & 0 \end{pmatrix} \xrightarrow{\textcircled{6}} c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix} \xrightarrow{\textcircled{7}} \mathrm{sgn}(\gamma_{\vec{w},\vec{u}})c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix}$$

$$H =: \sum c_{\vec{u}}\sigma_{\vec{u}}$$



①: Controllization

②, ③: Preparing blocks

④: Block-wise tracing

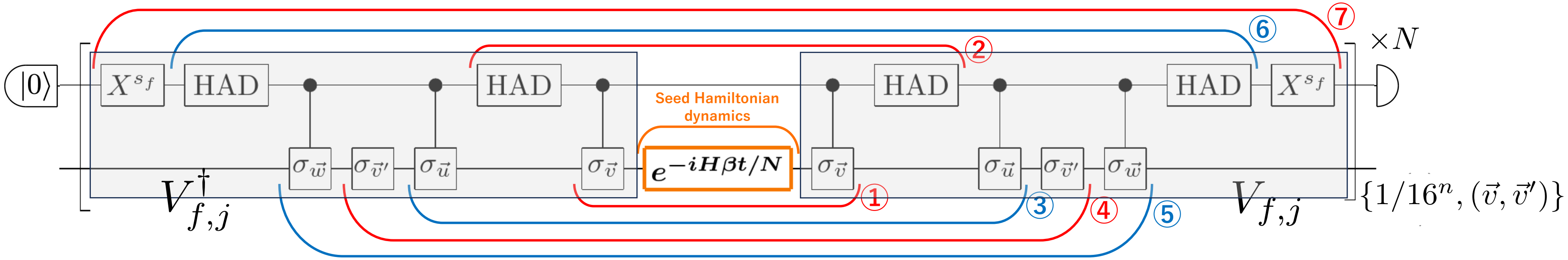
⑤, ⑥, ⑦: Basis change by Clifford

Detail of functional programming instance

$$I \otimes H = \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \xrightarrow{①} \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} \xrightarrow{②} \begin{pmatrix} H & H \\ H & H \end{pmatrix} \xrightarrow{③} \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix}$$

$$\xrightarrow{④} c_{\vec{u}} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \xrightarrow{⑤} c_{\vec{u}} \begin{pmatrix} 0 & \sigma_{\vec{w}} \\ \sigma_{\vec{w}} & 0 \end{pmatrix} \xrightarrow{⑥} c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix} \xrightarrow{⑦} \mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix}$$

$H =: \sum c_{\vec{u}} \sigma_{\vec{u}}$



①: Controllization

②, ③: Preparing blocks

④: Block-wise tracing

⑤, ⑥, ⑦: Basis change by Clifford

Description of function ① to ⑦

- Presentation slides are posted on our research group website

Slides are available here

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Application

We consider two applications:

- Negative time-evolution

- Hamiltonian single parameter learning

M. Quintino et al. PRL **123**, 210502 (2019), S. Yoshida et al. arXiv: 2209.02907 (2022)

Negative time-evolution

Linear map: $f(H) = -H$ $\qquad e^{-iHt} \mapsto e^{+iHt}$

- Applicable to block encoding of unknown Hamiltonian H given by $e^{-iH\tau}$

$$e^{-iH\tau}\ (\tau > 0) \mapsto U(H) := \begin{pmatrix} H & \cdot \\ \cdot & \cdot \end{pmatrix}$$

- Runtime is exponential in n in general, but when H has a sparse support, it can be polynomial (e.g. k-local)

S. Lloyd et al. arXiv: 2104.01410 (2021)

Hamiltonian single parameter learning

Linear map: $f_{\vec{v}}(H) = c_{\vec{v}}\underbrace{Y \otimes I \otimes \cdots \otimes I}_{\text{Rotation axis (arbitrary)}}$ $\qquad e^{-iHt} \mapsto e^{-i\underline{c_{\vec{v}}}Yt} \otimes I \otimes \cdots \otimes I$

$H =: \sum c_{\vec{u}}\sigma_{\vec{u}}$

Measure by QPE

- Total evolution time: $O(1/s)$ (Heisenberg limit)
- Runtime: $O(\|H\|_{\mathrm{op}}^2 n/s^2)$ $(\mathrm{poly}(n)$ for sparse $H)$

s : Allowed RMS of error

c.f. Heisenberg limit for restricted situation [4], Runtime of full tomography of e^{-iHt} [3]:
$O(\mathrm{poly}(\exp(n), 1/s))$

[3] S. Kimmel et al. PRA **92**, 062315 (2015), [4] H. Y. Huang, et al., Phys. Rev. Lett. 130, 200403 (2020).

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Higher-order transformation of Hamiltonian dynamics

Input:

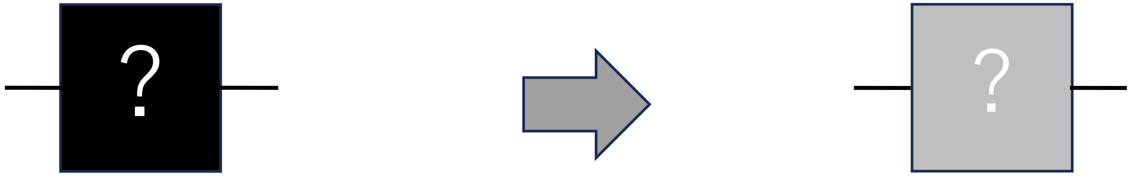
① Black-box dynamics

$e^{-iH\tau}\ (\tau > 0)$

Output:

Transformed dynamics

$e^{-if(H)t}$



② Function

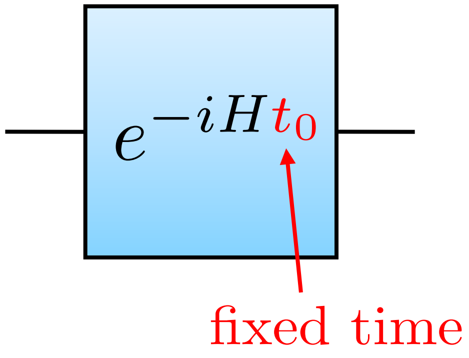
$H \mapsto f(H)$

Figure of merit: **Overall runtime**
(Not #queries to dynamics)

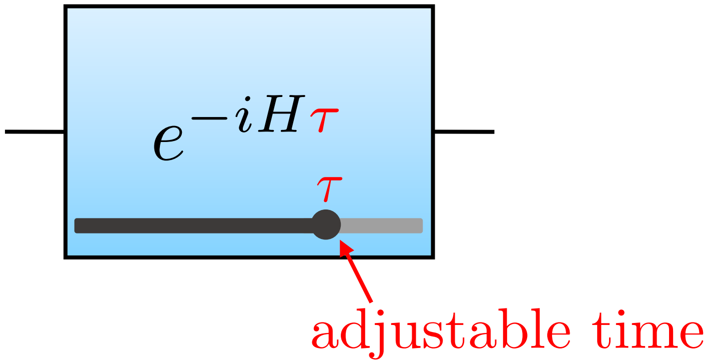
Difference with unitary input

Standard setting of higher-order transformation: black-box unitary input (e.g. inversion $U \mapsto U^\dagger$)

Unitary input



Hamiltonian dynamics input



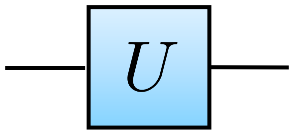
M. Quintino et al. PRL **123**, 210502 (2019), S. Yoshida et al. arXiv: 2209.02907 (2022)

Unitary input vs Hamiltonian dynamics input

Hamiltonian dynamics input has stronger simulatability

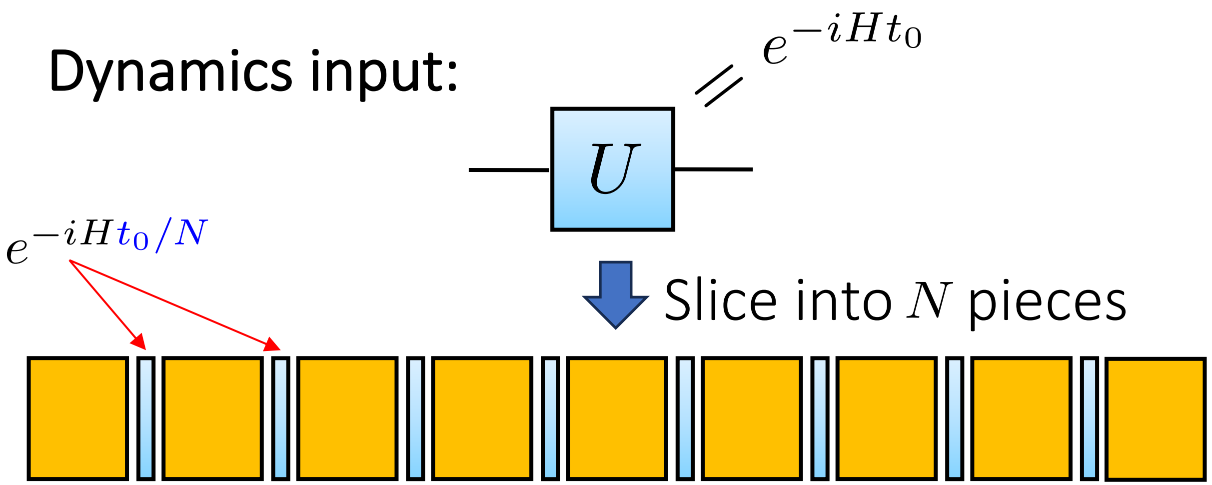
E.g. Controllization $U \mapsto \mathtt{ctrl}U$

Unitary input:



Impossible

Dynamics input:



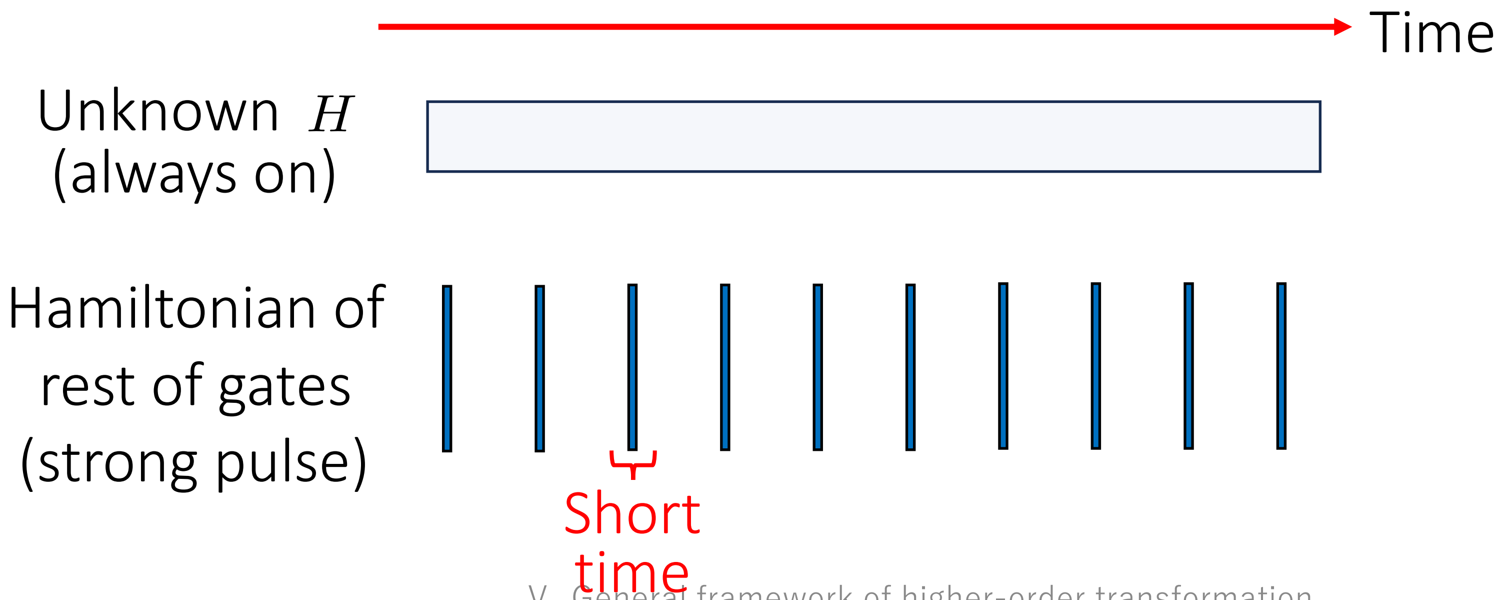
Possible

Z. Gavorova et al. arXiv:2011.10031 (2020). M. Araujo et al. New Journal of Physics 16, 093026 (2014). A. Soeda (Talk at IC- QIT, 2013). N. Friis et al. PRA **89**, 030303 (2014). Q. Dong et al. arXiv:1911.01645 (2019).

Practical implementation

The unknown dynamics can not be turned on/off in practice…

Fortunately, our algorithm can be approximately implemented if Clifford gates can be implemented in sufficiently short time



Summary

- We developed a new Hamiltonian simulation method applicable to simulation of unknown Hamiltonian
- Our algorithm can simulate $f(H)$ for an arbitrary physically realizable linear map f of Hamiltonian and unknown Hamiltonian H
- Part of our algorithm is developed by a quantum functional programming approach
- Our algorithm is an instance of higher-order transformations of Hamiltonian dynamics

Presentation slides

arXiv:2303.09788

Decomposition of linear functions

Arbitrary f can be decomposed into a sum of $\mathrm{sgn}(\gamma_{\vec{w},\vec{u}})f_{\vec{w},\vec{u}}$ with positive coefficients $|\gamma_{\vec{w},\vec{u}}|$

$$f = \sum_{\vec{u},\vec{w} \neq (0,\ldots,0)} |\gamma_{\vec{w},\vec{u}}| \cdot (\mathrm{sgn}(\gamma_{\vec{w},\vec{u}})f_{\vec{w},\vec{u}})$$

$$f_{\vec{w},\vec{u}} := \begin{array}{cc} & \vec{u} \\ \vec{w} & \begin{pmatrix} & 1 & \\ & & \\ & & \end{pmatrix} \end{array}$$

Mapping $\sigma_{\vec{u}}$ to $\sigma_{\vec{w}}$
(other input to 0)

Decomposition of linear functions

Arbitrary f can be decomposed into a sum of $\mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) f_{\vec{w},\vec{u}}$ with positive coefficients $|\gamma_{\vec{w},\vec{u}}|$

$$f = \sum_{\vec{u},\vec{w} \neq (0,\ldots,0)} |\gamma_{\vec{w},\vec{u}}| \cdot (\mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) f_{\vec{w},\vec{u}}) \qquad f_{\vec{w},\vec{u}} := \begin{array}{cc} & \begin{array}{ccc} & \vec{u} & \end{array} \\ \vec{w} & \begin{pmatrix} & 1 & \\ & & \\ & & \end{pmatrix} \end{array}$$

Can be simulated by summing $\mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) f_{\vec{w},\vec{u}}$ by random sampling

Decomposition of linear functions

Arbitrary f can be decomposed into a sum of $\mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) f_{\vec{w},\vec{u}}$ with positive coefficients $|\gamma_{\vec{w},\vec{u}}|$

$$f = \sum_{\vec{u},\vec{w} \neq (0,\ldots,0)} |\gamma_{\vec{w},\vec{u}}| \cdot (\mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) f_{\vec{w},\vec{u}}) \qquad f_{\vec{w},\vec{u}} := \begin{array}{cc} & \vec{u} \\ \vec{w} & \begin{pmatrix} & 1 & \\ & & \\ & & \end{pmatrix} \end{array}$$

Subgoal: Implementing $\mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) f_{\vec{w},\vec{u}} = \begin{array}{cc} & \vec{u} \\ \vec{w} & \begin{pmatrix} & \mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) & \\ & & \\ & & \end{pmatrix} \end{array}$ by

Hamiltonian simulation by random sampling

Simulation of one entry of PTM

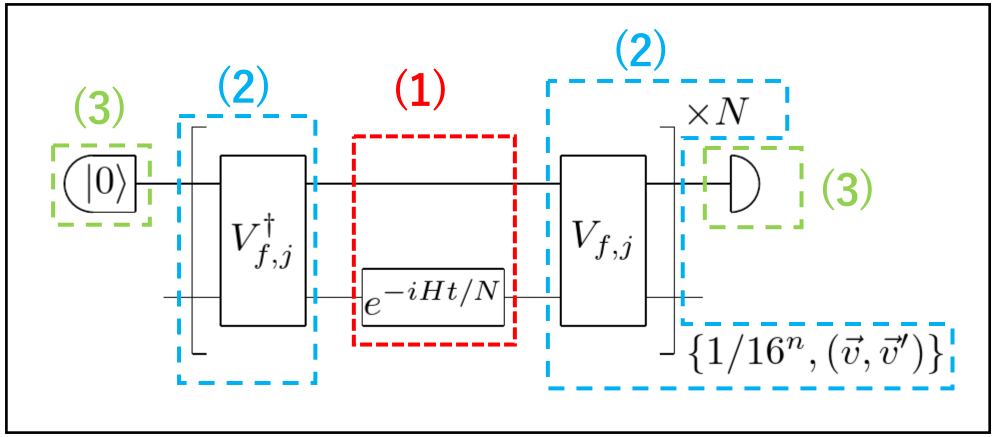
$H = \sum_{\vec{u} \neq (0,\ldots,0)} c_{\vec{u}} \sigma_{\vec{u}}$

$$H \xrightarrow{(1)} \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \xrightarrow{(2)} \begin{pmatrix} \mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) c_{\vec{u}} \sigma_{\vec{w}} & 0 \\ 0 & -\mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) c_{\vec{u}} \sigma_{\vec{w}} \end{pmatrix} \xrightarrow{(3)} \mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) \underline{c_{\vec{u}}} \sigma_{\vec{w}}$$

$$\mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) c_{\vec{u}} \sigma_{\vec{w}} = \mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) f_{\vec{w},\vec{u}}(H)$$

(1) Adding ancilla qubit

$$\underline{I} \otimes e^{-iHt} = \exp\left[-i \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} t \right]$$



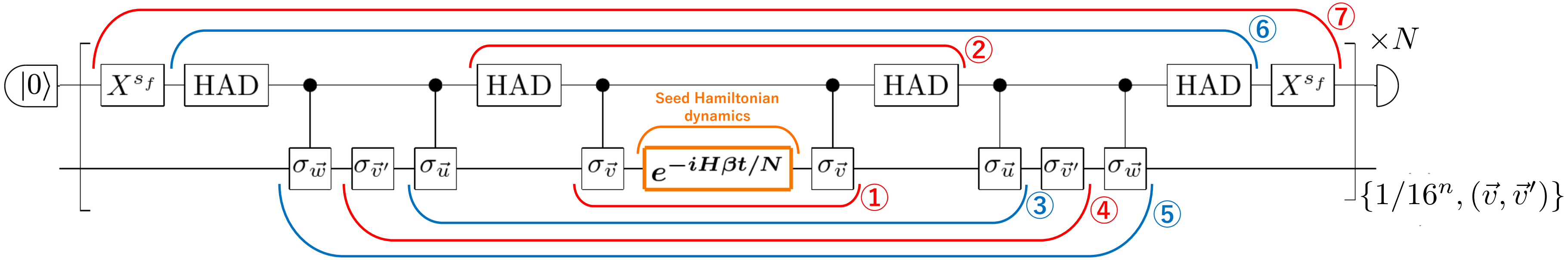
(3) Restricting ancilla to $|0\rangle$
(extracting top-left block)

Overview of Step (2)

$$I \otimes H = \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \xrightarrow{①} \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} \xrightarrow{②} \begin{pmatrix} H & H \\ H & H \end{pmatrix} \xrightarrow{③} \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix}$$

$$\xrightarrow{④} c_{\vec{u}} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \xrightarrow{⑤} c_{\vec{u}} \begin{pmatrix} 0 & \sigma_{\vec{w}} \\ \sigma_{\vec{w}} & 0 \end{pmatrix} \xrightarrow{⑥} c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix} \xrightarrow{⑦} \mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix}$$

$H =: \sum c_{\vec{u}} \sigma_{\vec{u}}$



$\mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) f_{\vec{w},\vec{u}}$ is constructed by concatenating function ①,...,⑦

Function ① (controllization)

$$I \otimes H = \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \xrightarrow{①} \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} \xrightarrow{②} \begin{pmatrix} H & H \\ H & H \end{pmatrix} \xrightarrow{③} \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix}$$

$$\xrightarrow{④} c_{\vec{u}} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \xrightarrow{⑤} c_{\vec{u}} \begin{pmatrix} 0 & \sigma_{\vec{w}} \\ \sigma_{\vec{w}} & 0 \end{pmatrix} \xrightarrow{⑥} c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix} \xrightarrow{⑦} \mathrm{sgn}(\gamma_{\vec{w},\vec{u}})c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix}$$

Sandwiching by random $\texttt{ctrl}\sigma_{\vec{v}}$

①: $$\sum_{\vec{v}\in\{0,1,2,3\}^n} \frac{1}{4^n} \begin{pmatrix} I & 0 \\ 0 & \sigma_{\vec{v}} \end{pmatrix} \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \sigma_{\vec{v}} \end{pmatrix}$$

$$= \underline{\begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix}} \qquad (H \text{ : traceless})$$

Gives $\begin{pmatrix} e^{-iHt} & 0 \\ 0 & I \end{pmatrix}$ when exponentiated

Q. Dong et al. arXiv:1911.01645 (2019).

Function ① (controllization)

$$I \otimes H = \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \xrightarrow{①} \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} \xrightarrow{②} \begin{pmatrix} H & H \\ H & H \end{pmatrix} \xrightarrow{③} \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix}$$

$$\xrightarrow{④} c_{\vec{u}} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \xrightarrow{⑤} c_{\vec{u}} \begin{pmatrix} 0 & \sigma_{\vec{w}} \\ \sigma_{\vec{w}} & 0 \end{pmatrix} \xrightarrow{⑥} c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix} \xrightarrow{⑦} \mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix}$$

Sandwiching by random $\texttt{ctrl}\sigma_{\vec{v}}$

①: $$\sum_{\vec{v} \in \{0,1,2,3\}^n} \frac{1}{4^n} \begin{pmatrix} I & 0 \\ 0 & \sigma_{\vec{v}} \end{pmatrix} \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \sigma_{\vec{v}} \end{pmatrix}$$

$$= \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix}$$ (H : traceless)

For Pauli $\sigma \in \{I, X, Y, Z\}^{\otimes n}$,

$$\frac{1}{4^n} \sum_{\vec{v} \in \{0,1,2,3\}^n} \sigma_{\vec{v}} \sigma \sigma_{\vec{v}} = \begin{cases} I & (\sigma = I) \\ 0 & (\text{otherwise}) \end{cases}$$

Function ②,③ (Preparing blocks)

$$I \otimes H = \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \xrightarrow{①} \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} \xrightarrow{②} \begin{pmatrix} H & H \\ H & H \end{pmatrix} \xrightarrow{③} \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix}$$

$$\xrightarrow{④} c_{\vec{u}} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \xrightarrow{⑤} c_{\vec{u}} \begin{pmatrix} 0 & \sigma_{\vec{w}} \\ \sigma_{\vec{w}} & 0 \end{pmatrix} \xrightarrow{⑥} c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix} \xrightarrow{⑦} \mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix}$$

Sandwiching by unitary (no randomness)

②: $2(\mathrm{HAD} \otimes I) \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} (\mathrm{HAD} \otimes I) = \begin{pmatrix} H & H \\ H & H \end{pmatrix}$

$\times 2$ is implemented only by doubling the simulation time

③: $\begin{pmatrix} I & 0 \\ 0 & \sigma_{\vec{u}} \end{pmatrix} \begin{pmatrix} H & H \\ H & H \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \sigma_{\vec{u}} \end{pmatrix} = \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix}$

Function ④ (block-wise tracing)

$$I \otimes H = \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \xrightarrow{①} \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} \xrightarrow{②} \begin{pmatrix} H & H \\ H & H \end{pmatrix} \xrightarrow{③} \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix}$$

$$\xrightarrow{④} c_{\vec{u}} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \xrightarrow{⑤} c_{\vec{u}} \begin{pmatrix} 0 & \sigma_{\vec{w}} \\ \sigma_{\vec{w}} & 0 \end{pmatrix} \xrightarrow{⑥} c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix} \xrightarrow{⑦} \mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix}$$

$H =: \sum c_{\vec{u}} \sigma_{\vec{u}}$

Sandwiching by random $\sigma_{\vec{v}'}$ on system

$$④: \sum_{\vec{v}' \in \{0,1,2,3\}^n} \frac{1}{4^n} (I \otimes \sigma_{\vec{v}'}) \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix} (I \otimes \sigma_{\vec{v}'})$$

$$= \begin{pmatrix} \mathrm{tr}(H)(I/2^n) & \mathrm{tr}(H\sigma_{\vec{u}})(I/2^n) \\ \mathrm{tr}(\sigma_{\vec{u}}H)(I/2^n) & \mathrm{tr}(\sigma_{\vec{u}}H\sigma_{\vec{u}})(I/2^n) \end{pmatrix}$$

$$\frac{1}{4^n} \sum_{\vec{v} \in \{0,1,2,3\}^n} \sigma_{\vec{v}} A \sigma_{\vec{v}} = \mathrm{tr}(A) \cdot \frac{I}{2^n}$$

Function ④ (block-wise tracing)

$$I \otimes H = \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \xrightarrow{①} \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} \xrightarrow{②} \begin{pmatrix} H & H \\ H & H \end{pmatrix} \xrightarrow{③} \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix}$$

$$\xrightarrow{④} c_{\vec{u}} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \xrightarrow{⑤} c_{\vec{u}} \begin{pmatrix} 0 & \sigma_{\vec{w}} \\ \sigma_{\vec{w}} & 0 \end{pmatrix} \xrightarrow{⑥} c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix} \xrightarrow{⑦} \mathrm{sgn}(\gamma_{\vec{w},\vec{u}})c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix}$$

$H =: \sum c_{\vec{u}}\sigma_{\vec{u}}$

Sandwiching by random $\sigma_{\vec{v}'}$ on system

$$④: \sum_{\vec{v}' \in \{0,1,2,3\}^n} \frac{1}{4^n}(I \otimes \sigma_{\vec{v}'}) \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix} (I \otimes \sigma_{\vec{v}'})$$

$$= \begin{pmatrix} \mathrm{tr}(H)(I/2^n) & \mathrm{tr}(H\sigma_{\vec{u}})(I/2^n) \\ \mathrm{tr}(\sigma_{\vec{u}}H)(I/2^n) & \mathrm{tr}(\sigma_{\vec{u}}H\sigma_{\vec{u}})(I/2^n) \end{pmatrix}$$

$$= \begin{pmatrix} 0 & c_{\vec{u}}I \\ c_{\vec{u}}I & 0 \end{pmatrix}$$

$$\mathrm{tr}(H) = \mathrm{tr}(\sigma_{\vec{u}}H\sigma_{\vec{u}}) = 0$$
$$\mathrm{tr}(H\sigma_{\vec{u}}) = \mathrm{tr}(\sigma_{\vec{u}}H) = 2^n c_{\vec{u}}$$

Function ⑤,⑥,⑦ (Basis change by Clifford)

$$I \otimes H = \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix} \xrightarrow{①} \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} \xrightarrow{②} \begin{pmatrix} H & H \\ H & H \end{pmatrix} \xrightarrow{③} \begin{pmatrix} H & H\sigma_{\vec{u}} \\ \sigma_{\vec{u}}H & \sigma_{\vec{u}}H\sigma_{\vec{u}} \end{pmatrix}$$

$$\xrightarrow{④} c_{\vec{u}} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \xrightarrow{⑤} c_{\vec{u}} \begin{pmatrix} 0 & \sigma_{\vec{w}} \\ \sigma_{\vec{w}} & 0 \end{pmatrix} \xrightarrow{⑥} c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix} \xrightarrow{⑦} \mathrm{sgn}(\gamma_{\vec{w},\vec{u}}) c_{\vec{u}} \begin{pmatrix} \sigma_{\vec{w}} & 0 \\ 0 & -\sigma_{\vec{w}} \end{pmatrix}$$

Sandwiching by unitary (no randomness)

⑤: $(\mathtt{ctrl}\sigma_{\vec{w}})(c_{\vec{u}}X \otimes I)(\mathtt{ctrl}\sigma_{\vec{w}}) = (c_{\vec{u}}X \otimes \sigma_{\vec{w}})$

⑥: $(\mathrm{HAD} \otimes I)(c_{\vec{u}}X \otimes \sigma_{\vec{w}})(\mathrm{HAD} \otimes I) = (c_{\vec{u}}Z \otimes \sigma_{\vec{w}})$

⑦: $(X^{s_f} \otimes I)(c_{\vec{u}}Z \otimes \sigma_{\vec{w}})(X^{s_f} \otimes I) = \mathrm{sgn}(\gamma_{\vec{w},\vec{u}})(c_{\vec{u}}Z \otimes \sigma_{\vec{w}})$ $\qquad s_f := (1 - \mathrm{sgn}(\gamma_{\vec{w},\vec{u}}))/2$

1. Hamiltonian simulation with random sampling

Sum and concatenation of transformations of shape $H \mapsto \sum_j h_j U_j H U_j^\dagger$ can also be simulated using random sampling

$$f(H) := \sum_j h_j \left(U_j H U_j^\dagger\right)$$

$$g(H) := \sum_k r_k \left(V_k H V_k^\dagger\right)$$

Sum $\alpha f + \beta g \ (\alpha, \beta > 0)$

① choose f or g in prob. $\alpha/(\alpha+\beta)$ and $\beta/(\alpha+\beta)$

② choose $\begin{cases} U_j & (f \text{ is chosen}) \\ V_k & (g \text{ is chosen}) \end{cases}$ with prob. $\begin{cases} h_j/\sum_j h_j \\ r_k/\sum_k r_k \end{cases}$

Concatenation $g \circ f$

Choose $V_k U_j$ with prob. $(h_j/\sum_j h_j)(r_k/\sum_k r_k)$

2. Pauli transfer matrix (PTM)

We describe n-qubit case:

$$H = \sum_{\vec{u}} c_{\vec{u}} \sigma_{\vec{u}} \Leftrightarrow \begin{pmatrix} 0 \\ c_{(0,\ldots,1)} \\ \vdots \\ c_{(3,\ldots,3)} \end{pmatrix} \in \mathbb{R}^{4^n}$$

$$\sigma_{\vec{v}} := \sigma_{v_1} \otimes \cdots \otimes \sigma_{v_n}$$

Hermitian preserving linear map f

$$\text{s.t. } f(\sigma_{\vec{u}}) = \sum_{\vec{w}} \gamma_{\vec{w},\vec{u}} \sigma_{\vec{w}} \Leftrightarrow$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \gamma_{(0,\ldots,1),(0,\ldots,1)} & \cdots & \gamma_{(0,\ldots,1),(3,\ldots,3)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \gamma_{(3,\ldots,3),(0,\ldots,1)} & \cdots & \gamma_{(3,\ldots,3),(3,\ldots,3)} \end{pmatrix}$$

PTM of “physically realizable linear map”

First row/column of PTM can w.l.o.g taken to be 0 (otherwise unphysical)