# From noncommutative optimal transport to limitations of quantum simulation

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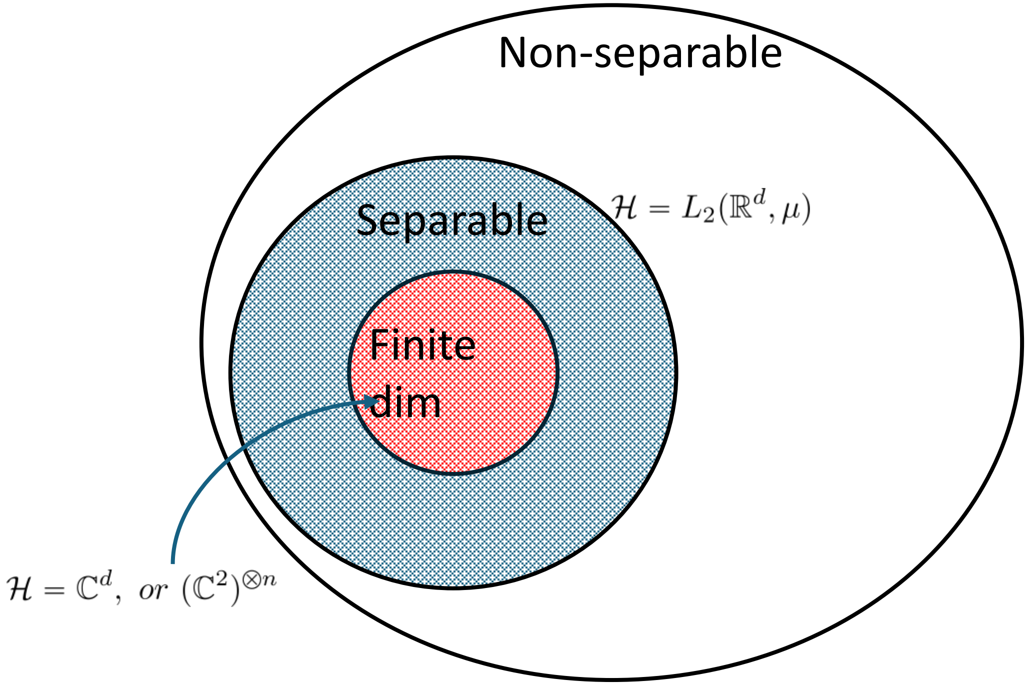
+ Discussion at IPAM

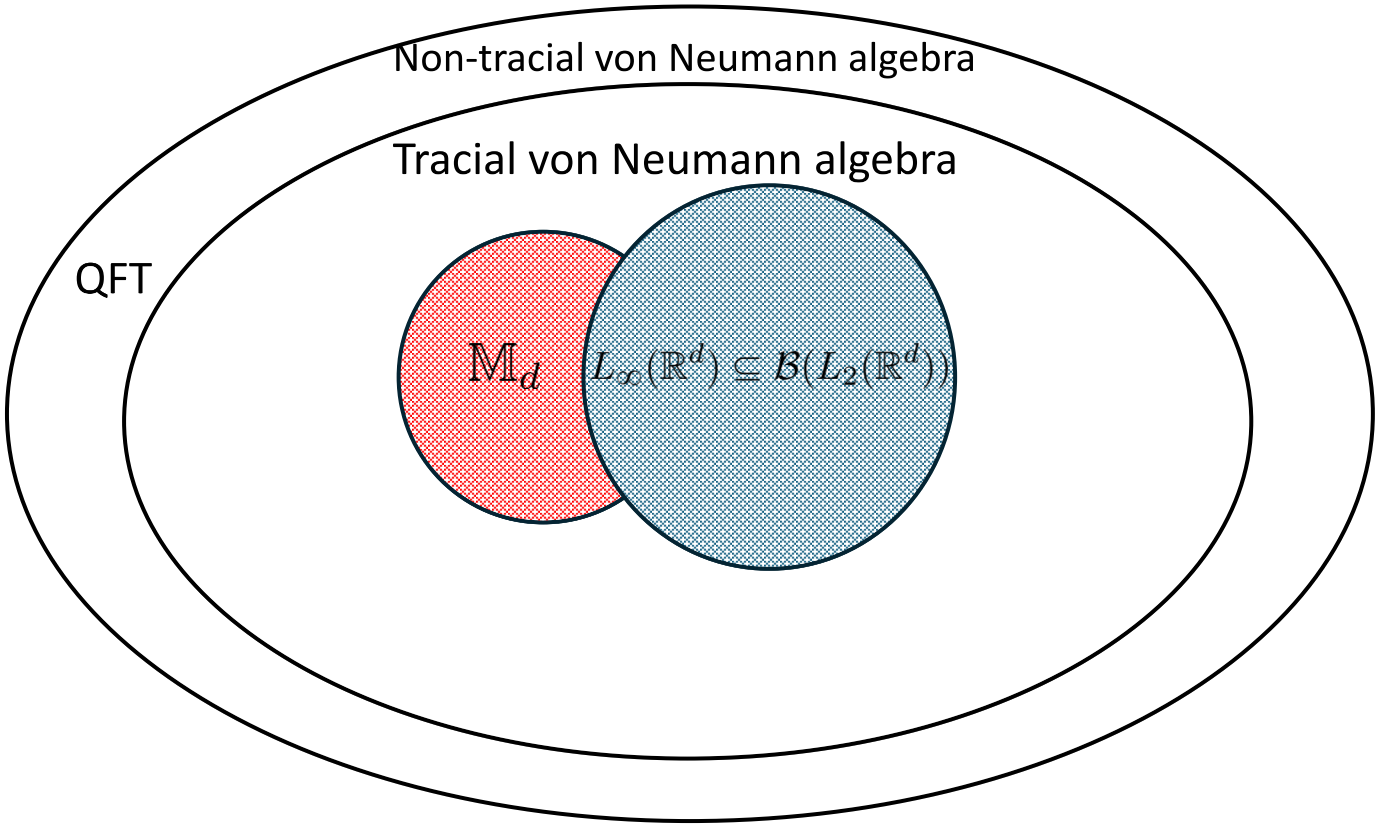
+ Discussion inside Junge team

# Which Hilbert space do I live in?

We are living in a “Hilbert space” doing “algebra”




Hierarchy of Hilbert space




Hierarchy of algebras

# Optimal transport theory

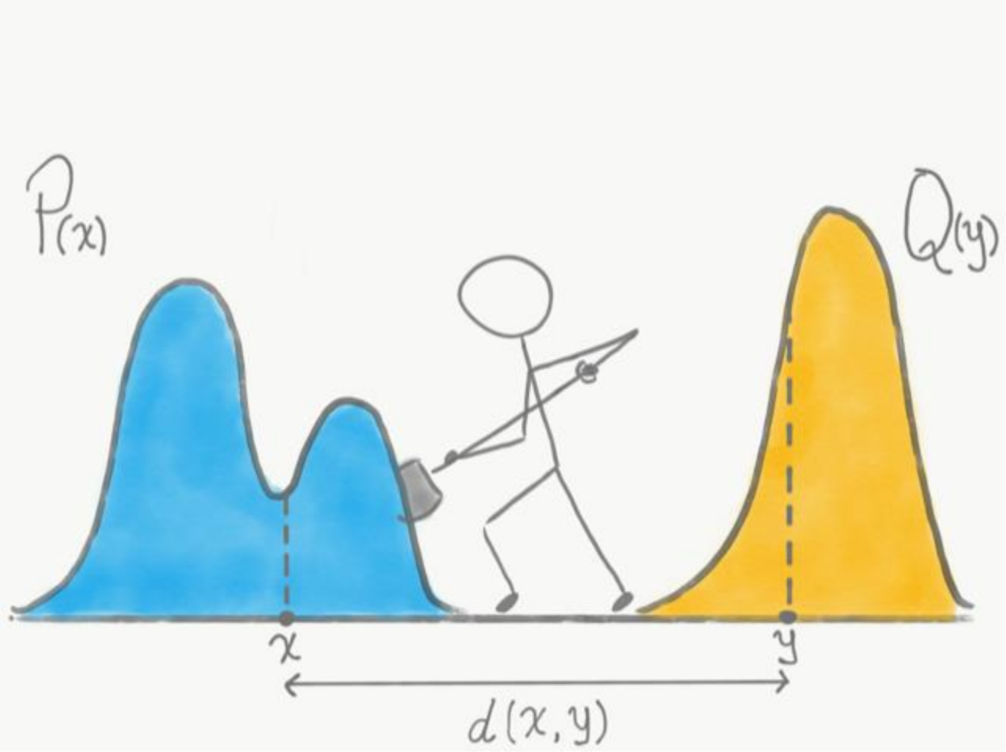
- What is the least “work” needed to reshape one probability distribution(state) into another?
- In the noncommutative setting, states are density operators(positive with trace 1) on a Hilbert space.
- Monge-Kantorovich transportation cost

$$\mathcal{T}(\rho,\sigma) = \inf_{\Pi \in \mathfrak{C}'(\rho,\sigma)} \mathrm{Tr}(C\Pi)$$

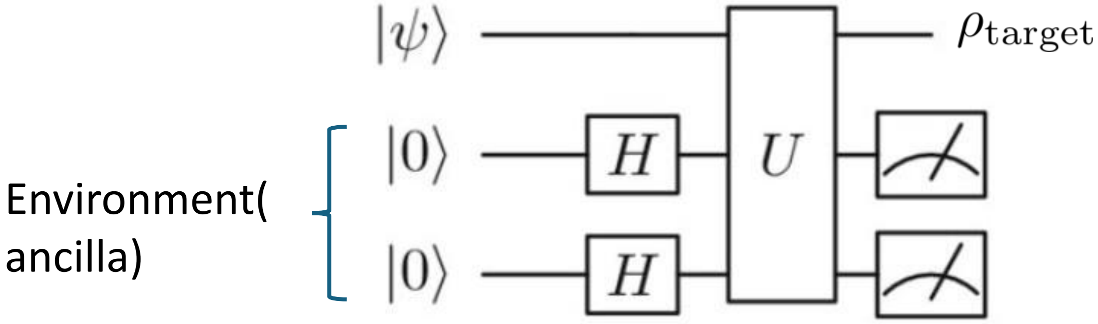
$\mathfrak{C}'(\rho,\sigma)$: a subset of couplings of $\rho, \sigma$.
$C$: a cost operator.

$$\mathcal{T}(\rho,\sigma) = \sup_{(A,B)\in\mathcal{B}_c} |\mathrm{Tr}(\rho A) - \mathrm{Tr}(\sigma B)|$$

$\mathcal{B}_c \subseteq \mathcal{B}(\mathcal{H}) \times \mathcal{B}(\mathcal{H})$: a suitably chosen dual pairs



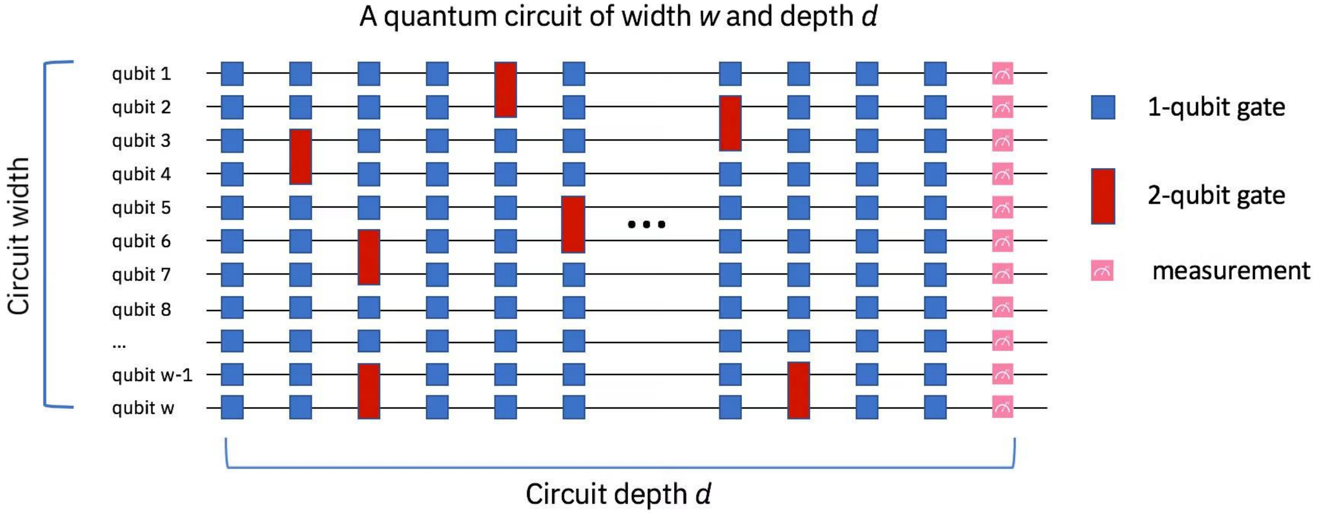
# Quantum simulation




$$\mathrm{Count}(U) = \min\{l \geqslant 1 : U = u_1 u_2 \cdots u_l, u_i \in S\}.$$

- Given an initial "easy" state and a target state, what is the minimal number of unitary operators to transform one to another?
- S is a set of "cheap" unitary operators
- A realistic case is the set S consists of
- each unitary touches only a few qubits

$V = \bigotimes_j U_j$




$$\mathrm{Depth}(U) = \min\{l \geqslant 1 : U = V_1 \cdots V_l, V_i = \bigotimes_j U_j, U_j \text{ is } k-\text{local}\}.$$

# Lower bound on quantum simulation: a summary

- Commutator (Triangle inequality) bound
- Geometric (Nielsen) approach: Geodesic length.
- Volume and covering arguments
- Schmidt-rank: lower bound on depth
- Lieb-Robinson velocity(continuous setting) and light cone argument(discrete setting)

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**This work!**

# Connection

- We show that the minimal number of gates or depth for a quantum simulation task can be lower bounded by the transportation cost, with the dual picture given by Connes 1989, Rieffel 2003.

The key ingredient is the commutator $[A, B] := AB - BA$, and the Lipschitz semi-norm

$$|||A|||_S := \sup_{s \in S} \|[s, A]\|_{op}. \tag{1}$$

The transportation cost from $\rho$ to $\sigma$ is defined by

$$W_S(\rho, \sigma) = \sup_{|||A|||_S \leqslant 1, A = A^\dagger} \mathrm{Tr}(\rho A) - \mathrm{Tr}(\sigma A) \tag{2}$$

## Exercise 1

$$\mathrm{Count}(U) := \min\{l \geqslant 1 : U = u_1 u_2 \cdots u_l, u_i \in S\}.$$

$$\mathrm{Count}(U) \geqslant \frac{\|[U, x]\|_{op}}{\sup_{u \in S} \|[u, x]\|_{op}}, \quad x \in \mathcal{B}(\mathcal{H}).$$

It is a well-known commutator triangle inequality. Suppose $U = u_1 \cdots u_l$, using the Leibniz rule for commutators, $[AB, C] = A[B, C] + [A, C]B$, and triangle inequalities,

$$\begin{aligned}
\|[u_1 \cdots u_l, x]\|_{op} &\leqslant \|u_l [u_{l-1} \cdots u_1, x]\|_{op} + \|[u_l, x] u_{l-1} \cdots u_1\|_{op} \\
&\leqslant \|[u_{l-1} \cdots u_1, x]\|_{op} + \|[u_l, x]\|_{op} \\
&\leqslant \sum_{i=1}^{l} \|[u_i, x]\|_{op} \leqslant l \sup_i \|[u_i, x]\|_{op}.
\end{aligned}$$

## Exercise 2

$$\mathrm{Depth}(U) = \min\{l \geqslant 1 : U = V_1 \cdots V_l, V_i = \bigotimes_j U_j, U_j \text{ is } k-\text{local}\}.$$

Suppose $S$ is the set of 1-local Pauli operators.

$$(2k)^{\mathrm{Depth}(U)} \geqslant \frac{\sup_{P\in S} \|[P, U^\dagger x U]\|_{op}}{\sup_{P\in S} \|[P, x]\|_{op}}, \forall x \in \mathcal{B}(\mathcal{H}).$$

For any $P \in S$, $V = \bigotimes_j U_j$, we have

$$\begin{aligned}
\|[P, V^\dagger x V]\|_{op} &= \|[VPV^\dagger, x]\|_{op} \\
&= \|[U_j P U_j^\dagger, x]\|_{op}, \ U_j \text{ is } k-\text{local} \\
&= \|[U_j P U_j^\dagger, x - \mathrm{tr}_k(x) \otimes \mathbb{I}_k/2^k]\|_{op} \\
&= \|[P, U_j^\dagger(x - \mathrm{tr}_k(x) \otimes \mathbb{I}_k/2^k)U_j]\|_{op} \\
&\leqslant 2\|PU_j^\dagger(x - \mathrm{tr}_k(x) \otimes \mathbb{I}_k/2^k)U_j\|_{op} \\
&= 2\|x - \mathrm{tr}_k(x) \otimes \mathbb{I}_k/2^k\|_{op} \\
&= 2\|\frac{1}{2^k}\sum_{P_k\in S_k}(x - P_k x P_k)\|_{op} \\
&\leqslant 2\sup_{P_k\in S_k}\|[P_k, x]\|_{op} \leqslant 2k\sup_{P\in S}\|[P, x]\|_{op}
\end{aligned}$$

$S_k$ is the set of $k$-local Pauli operators.

$$\|[P_k, x]\|_{op} \leqslant k \sup_{P\in S}\|[P, x]\|_{op}.$$

Apply the inequality $l$ times,

$$\|[P, (V_1\cdots V_l)^\dagger x (V_1 \cdots V_l)]\|_{op} \leqslant (2k)^l \sup_{P\in S}\|[P, x]\|_{op}.$$

# Two quantities

- Motivated by the previous calculations, we introdu the following quantities for quantum circuits, or m generally, quantum channels.

$$\mathrm{Cost}_S(\Phi) := \sup_{x=x^\dagger, |||x|||_S \leqslant 1} \|\Phi^*(x) - x\|_{op}, \tag{1}$$

$$\mathrm{Lip}_S(\Phi) := \sup_{x=x^\dagger, |||x|||_S \leqslant 1} |||\Phi^*(x)|||_S. \tag{2}$$

The first quantity, called transportation cost of channels(also named as Lipschitz cost), provides a lower bound on the volume(number of unitary operators). The second quantity, called Lipschitz constant, provides a lower bound on the depth.

# Wasserstein metric

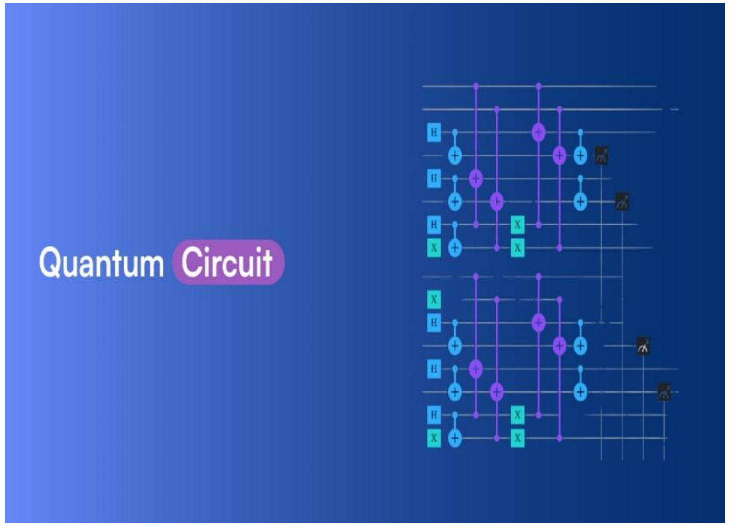
The first quantity is the maximal cost from any state to $\Phi$. The second quantity is the contraction coefficient under the Wasserstein metric.

$$\mathrm{Cost}_S(\Phi) := \sup_{\rho} W_S(\rho, \Phi(\rho)), \tag{1}$$

$$\mathrm{Lip}_S(\Phi) := \sup_{\rho \neq \sigma} \frac{W_S(\Phi(\rho), \Phi(\sigma))}{W_S(\rho, \sigma)}. \tag{2}$$

# Limitations on simulation of Lindblad dynamics

**Strong quantum Church-Turing thesis:**
*Every quantum mechanical computational process can be simulated efficiently in the unitary circuit model of quantum computation.*




Lindbladian generator:

$$L(\rho) = \underbrace{-i[H,\rho]}_{\text{coherent part}} + \sum_{j=1}^{m} \underbrace{L_{V_j}(\rho)}_{\text{dissipative part}} \quad , \; L_V(\rho) = \underbrace{V\rho V^\dagger}_{\text{Jump}} - \frac{1}{2}\underbrace{(V^\dagger V\rho + \rho V^\dagger V)}_{\text{No jump}} .$$

**Q: Given a set of accessible unitary circuits (gates), what is the minimum number of gates (simulation cost) required to approximate an open quantum system at a target time T?**

# Preparing Gibbs state via Lindbladians

Given a Hamiltonian on $n$-qubit system, how do we design a Lindbladian such that it converges to the Gibbs state

$$\rho_\beta = \frac{\exp(-\beta H)}{\mathrm{Tr}(\exp(-\beta H))}, \beta \in (0, \infty)$$

Idea: design a Lindbladian admitting the Gibbs state as the unique fixed state. To ensure mixing fast, we assume symmetry property.

# Gibbs state sampler: KMS and GNS symmetry

- There are two typical choices for the Gibbs sampler:
- GNS symmetry:

$$\mathrm{Tr}(\rho_\beta \mathcal{L}_\beta(X) Y) = \mathrm{Tr}(\rho_\beta X \mathcal{L}_\beta(Y)).$$

- KMS symmetry:

$$\mathrm{Tr}\left(\rho_\beta^{1/2} \mathcal{L}_\beta(X) \rho_\beta^{1/2} Y\right) = \mathrm{Tr}\left(\rho_\beta^{1/2} X \rho_\beta^{1/2} \mathcal{L}_\beta(Y)\right).$$

# The issue with GNS Gibbs sampler

- GNS detailed balance is equivalent to the Lindbladian generator commuting with the modular automorphism group:

$$\sigma_t^{\rho_\beta}(X) := \rho_\beta^{it} X \rho_\beta^{-it}.$$

- The jump operators must be the eigen-operators of the modular automorphism group (see the remark in Carlen-Maas).
- Physically, it means the dissipation channel must “know about” the entire spectrum of the Hamiltonian.
- By energy-time uncertainty principle, it requires exponential time to implement.

# Why KMS Gibbs sampler is a remedy

- Recall that a Lindbladian generator satisfies KMS-symmetry, if and only if

$$\mathcal{L}(X) = i[G, X] + \sum_j L_{V_j},$$

$$\Delta_\sigma^{1/2}(V_j) = V_j^\dagger \text{ and}$$

$$G = -i \tanh\Big(\log\Big(\Delta_\sigma^{1/4}\Big)\Big)\Big(\frac{1}{2}\sum_j V_j^\dagger V_j\Big).$$

# KMS Gibbs sampler

- To design a KMS Gibbs sampler, we choose the jump operator as

$$V_j = \int_0^\infty f_\beta(t) \exp(iHt)\sigma_j \exp(-iHt) dt, \tag{1}$$

  here $\sigma_j$ is the set of single Pauli gates
- The function is a nicely chosen function, usually Gaussian type.
- We choose the Hamiltonian part to make sure the Lindbladian is KMS symmetric. Implementing this Lindbladian only needs Hamiltonian evolution + energy-gap filters which have polynomially many circuits.

# Theorem(Ding, Junge, Schleich, W.): Limitations of this simulation algorithm

- Using the Hamiltonian and energy-gap filters, when the temperature is very high, any simulation algorithm must incur a simulation cost satisfying

$$\mathrm{Cost}(T_t) \geqslant c \cdot t\left(\lambda_{\max}(H) - \lambda_{\min}(H)\right)$$

  for small constant time t and universal constant $c > 0$.
- Our method is restrictive to rapid mixing dynamics.
- When the temperature is very low, B. Kiani's talk in workshop I showed that the mixing time is slow.
- Modified Log-Sobolev inequality is completely open: find a non-GNS and KMS-symmetric Lindbladian admitting the Gibbs state of a non-commuting Hamiltonian as the fixed state, such that MLSI fails.
- An alternative approach for mixing time is

$$\mathrm{Lip}(T_t) \leqslant c\exp(-\lambda t)$$

# lower bound on the depth of a quantum channel

Suppose $\Phi$ is a quantum channel on $\mathcal{B}\left(\bigotimes_{i=1}^{n} \mathcal{H}_i\right)$ of layer $L$

$$\Phi = \prod_{\ell=1}^{L} \Phi_\ell.$$

Then for any resource set, $S^n \subseteq \mathcal{B}\left(\bigotimes_{i=1}^{n} \mathcal{H}_i\right)$ we have

$$L \geqslant \frac{\log\left(\mathrm{Lip}_{S^n}(\Phi)\right)}{\log\left(\max_{1\leqslant \ell \leqslant L} \mathrm{Lip}_{S^n}(\Phi_\ell)\right)}.$$

# A concrete lower bound on the Lipschitz constant by measurement on the output state

- In $n$-qubit system with orthonormal basis

$$\{|\psi_x\rangle\}_{x\in\mathcal{X}}, \text{ where } \mathcal{X} = \{0,1\}^n \text{ and } S^n \subseteq \mathcal{B}(\mathcal{H}).$$

- Initial state: $\rho_{in}$; output state: $\sigma = \Phi(\rho_{in})$.

- Define $$\mu_\sigma(x) = \langle\psi_x|\, \sigma\, |\psi_x\rangle, \quad x \in \mathcal{X}. \tag{1}$$

- Note that in the literature, the orthonormal basis is chosen as the computational basis. Here we do not assume that.

# Main result(DJSW25+)

- If $\Phi$ is a circuit, then the Lipschitz constant of $\Phi$ must satisfy

$$\mathrm{Lip}_{S^n}(\Phi) \geqslant \frac{\min_{x\in A, y\in B} |f(x) - f(y)|}{|||O_f|||_{S^n}} \times \frac{1}{\left(\mu_\sigma(A)^{-\frac{1}{2}} + \mu_\sigma(B)^{-\frac{1}{2}}\right)\sqrt{Poinc_2(\rho_{in})}},$$

  for any $A, B$ *and* $f$. $$Poinc_2(\rho) = \sup_{|||O|||_{S^n} \leqslant 1} \mathrm{tr}\left(\rho O^2 - \mathrm{tr}(\rho O)^2\right)$$

- Note that if we choose the orthonormal basis as the computational basis, it recovers the well-known Harrow-Lidar argument (well-spread property for the output state).
- Answering a question during M. Marvian's talk.

# Reference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