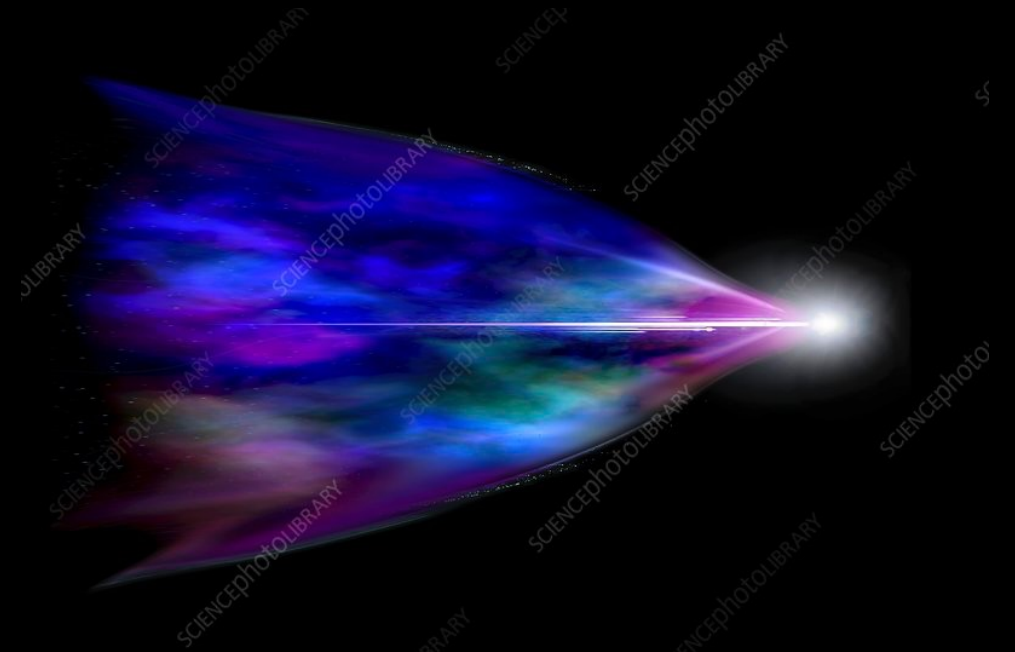


Lieb-Robinson bound and its applications

1



Tomotaka Kuwahara
RIKEN, RQC & CPR



Self-introduction

- U. Tokyo (-2015.3) → JPSJ PD → AIMR, Tohoku U. Assistant Prof. (2016-2017.9)
→ RIKEN AIP (2017.10-2022.3) → RIKEN Hakubi (2022.4-)
- My interest: mathematics connecting condensed matter, many-body physics, quantum computation
Area law conjecture or Quantum PCP conjecture
J. Eisert, et al., Rev. Mod. Phys. (2010) D. Aharonov, I. Arad, T. Vidick, AcM SIGACT News (2013)
- Floquet theory: Ann. Phys. 367, 96 (2016), PRL 116, 120401 (2016), PRL 120, 220602 (2018)
- Area law : Nature Communications 11, 4478 (2020), PRX 11, 011047 (2021)
- Entanglement at finite temperatures: PRL 124, 220601 (2020), PRX 12, 021022 (2022)
- Lieb-Robinson bound:** PRX 10, 031010 (2020), PRL 126, 030604 (2021), PRL 127, 070403 (2021)
- Hamiltonian learning: Nature Physics volume 17, pages 931–935 (2021)

Main purpose

- Elementary introduction to Hamiltonian Complexity
- Basics of the Lieb-Robinson bound
- Applications of the Lieb-Robinson bound (e.g., clustering theorem)
- Very recent progresses
(entanglement clustering, bosonic Lieb-Robinson bound)

Elementary introduction of Hamiltonian Complexity

Summary:

Hamiltonian complexity aims to clarify information-theoretic structures of quantum many-body systems

Quantum Computer

5



0 1



0 + 1



Much faster computer ?
→ Shor's factorization algorithm

PW Shor, SIAM review, 1999



Google's experiment

- Random circuit sampling

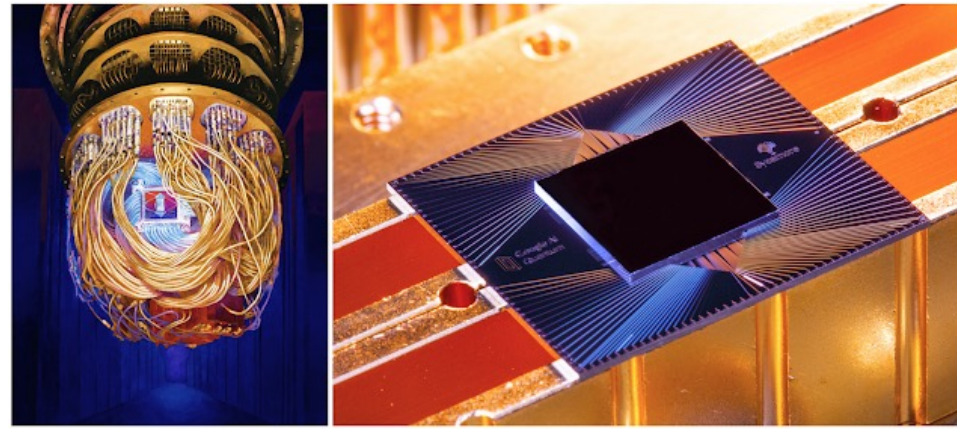
→ Difficult by classical computers

F. Aruta, et al., Nature (2019)

10000 years by classical computers

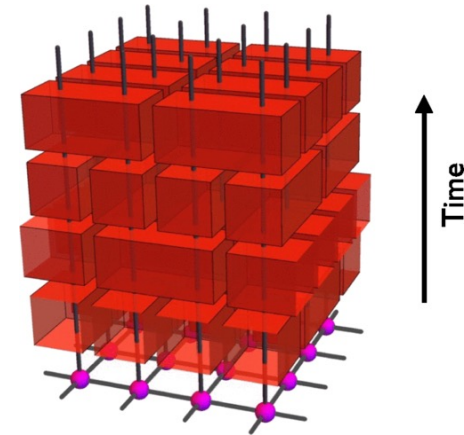
→ 200 seconds by a quantum computer

1,500,000,000 times faster !!



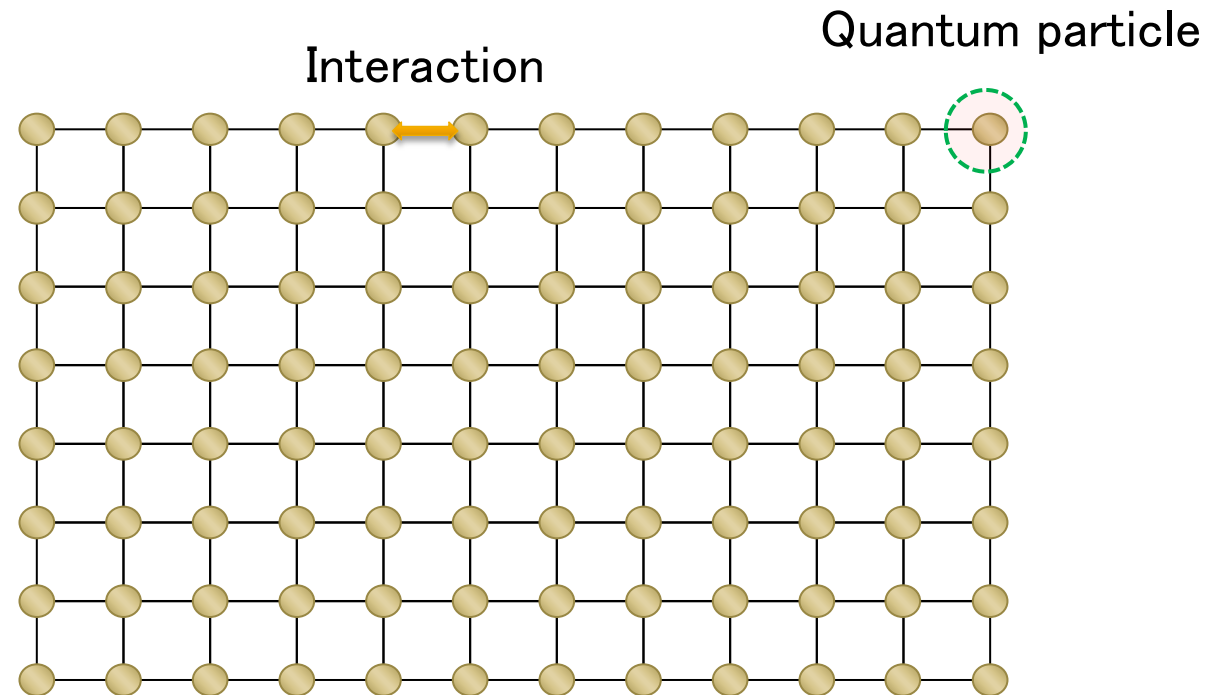
Sycamore by Google

53 qubits,
qubit: quantum unit for computational use



But, random circuit sampling is useless in practical applications...

Quantum many-body physics



Can we efficiently compute properties of quantum many-body systems?

Hamiltonian Complexity

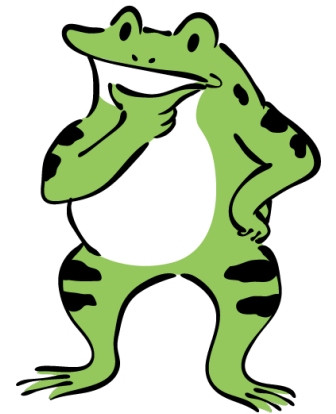
- **Hamiltonian**: all the information on the many-body system

$$\frac{d}{dt}|\psi(t)\rangle = -iH|\psi(t)\rangle \quad : \text{Schrödinger equation} \quad H: \text{Hamiltonian}$$

- How difficult is it to compute properties of a Hamiltonian?
(e.g., the lowest energy states)

→ QMA complete ($\Leftrightarrow$ NP complete in classical computation)

→ In general, no efficient algorithm even by quantum computers !





Hamiltonian Complexity

Q. In what cases can we efficiently simulate the quantum Hamiltonian?

Computer science



quantum many-body physics



Useful ???

Is it related to practically important problems, e.g., machine learning ?

Hamiltonian Complexity

Most of the practically interesting problems (QMA class)

→ quantum many-body problems
reduce

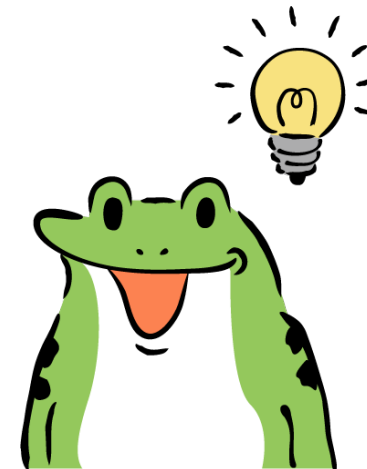


← **Target !**

Efficient algorithm



Practical applications (e.g., semi-definite programming)





Semi-definite programming (SDP)

Vandenberghe and Boyd, SIAM Review, 38(1), 49–95 (1996), GRG Lanckriet, et al., Journal of Machine Learning Research 5 (2004) 27–72, F. Alizadeh, SIAM journal on Optimization, 5(1), 13–51 (1995), A. d'Aspremont, et al., SIAM Review, 49(3), 434–448 (2007)

SDP: One of the most important optimization problems

[Input] $\{C, A_1, A_2, \dots, A_m\}$: $N \times N$ Hermitian matrices $\longrightarrow$ [Problem] X : $N \times N$ semidefinite matrix

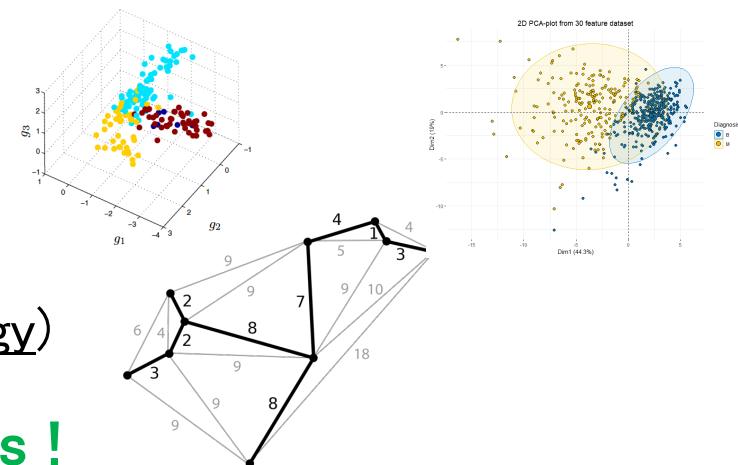
$\{b_1, b_2, \dots, b_m\}$: real numbers

Constraints: $\text{tr}(X A_j) \leq b_j \quad j = 1, 2, \dots, m$

Calculation: $\max_{X: X \succeq 0} [\text{tr}(CX)]$

reduce

- Kernel-based machine learning ($\leftarrow$ support vector machine)
- Combinatorial optimization ($\leftarrow$ operational research)
- Principal component analysis ($\leftarrow$ data analysis, finance, biology)



Various industrial applications !

★ Quantum algorithm achieves an exponential speed up if quantum Gibbs sampling is efficiently performed ! Brandao and Svore (FOCS'17)

A main target of the Hamiltonian complexity !!

Several crucial problems

★ Various problems are mathematically well-defined!

Quantum Gibbs sampling, SDP

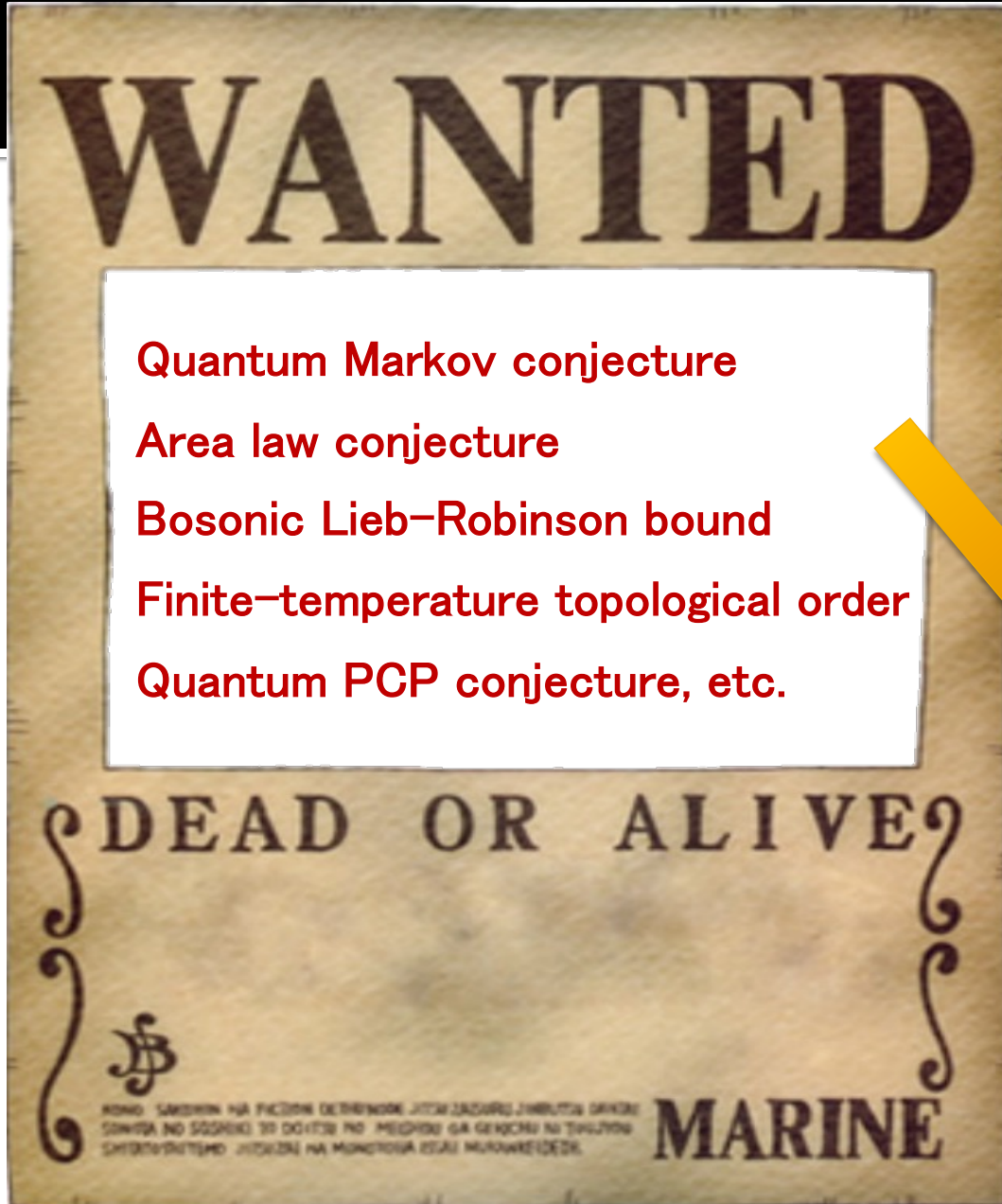
Density Matrix Renormalization Group method

Quantum simulator

Fault tolerant quantum computation

Foundation of quantum computing

Identifying the universal aspects of generic many-body systems!



Recently solved!

Quantum Markov
Area law conjecture

Bosonic Lieb–Robinson bound

Finite-temperature topological order

Quantum PCP conjecture, etc.

Several crucial problems

★ Various problems are mathematically well-defined!

Quantum Gibbs sampling, SDP

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Quantum Markov
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Quantum PCP conjecture, etc.

★ Various problems are mathematically well-defined!

Quantum Gibbs sampling, SDP

Density Matrix Renormalization Group method

A weaker version (No-Low-Energy-Trivial State Conjecture) has been proved...

Anshu, Breuckmann, Nirkhe, arXiv:2206.13228

m computation

m computing

**versal aspects of
generic many-body systems!**

Basics of the Lieb-Robinson bound

1 : Motivation

Summary:

Quantifying the speed limit to generate correlations by many-body dynamics

Motivation: quantum time evolution

- Schrödinger equation for time dependent Hamiltonian

$$\frac{d}{dt}|\psi(t)\rangle = -iH(t)|\psi(t)\rangle$$

$$|\psi(t)\rangle = \mathcal{T}[e^{-i \int_0^t H(t)dt}]|\psi(0)\rangle$$

Time ordering operator

Time evolution operator

$$\mathcal{T} \left[e^{-i \int_0^t H(t)dt} \right] := \lim_{n \rightarrow \infty} e^{-i \frac{t}{n} H(t_n)} e^{-i \frac{t}{n} H(t_{n-1})} \dots e^{-i \frac{t}{n} H(t_2)} e^{-i \frac{t}{n} H(t_1)}$$

We want to calculate it !

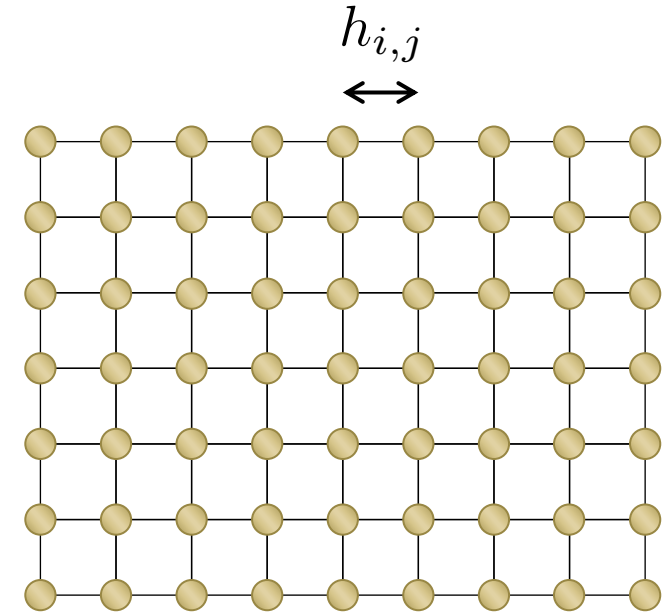
$$t_m := \frac{mt}{n}$$

Dimension of Hilbert space

- (1/2)-spin system (nearest neighbor interaction)

$$H = \sum_{\langle i,j \rangle} h_{i,j}$$

e.g., $H = \sum_{\langle i,j \rangle} J(\sigma_i^x \otimes \sigma_j^x + \sigma_i^y \otimes \sigma_j^y + \sigma_i^z \otimes \sigma_j^z)$



- Dimension of Hilbert space $= 2^n$ (n : number of spins)
- Time evolution operator $\mathcal{T}[e^{-i \int_0^t H(t) dt}] : 2^n \times 2^n$ matrix
- ➡ ($n = 20$) $10^6 \times 10^6$ matrix !

Approximation of dynamics

- Why is the calculation difficult?



- Principle of superposition

$$a_1 |\overbrace{000 \cdots 0}^N\rangle + a_2 |010 \cdots 0\rangle + a_3 |110 \cdots 0\rangle + a_4 \cdots$$

Ignoring the spin-spin correlations



So bad precision...

- Mean-field approximation : approximate by the product state

$$|\psi(t)\rangle \longrightarrow |\psi_1(t)\rangle \otimes |\psi_2(t)\rangle \otimes |\psi_3(t)\rangle \otimes \cdots \otimes |\psi_N(t)\rangle$$

Problems

- Mean-field approximation: ignoring the correlation completely

Bad precision



Can we approximate the dynamics with good accuracy by incorporating a “moderate amount” of correlations?

- Rigorous diagonalization: taking all the correlations into account

Solvable only for small systems (~ 20 spins)

Problems

- Mean-field approximation: ignore correlations

Bad precision

We need to know how much correlation is generated by the dynamics !

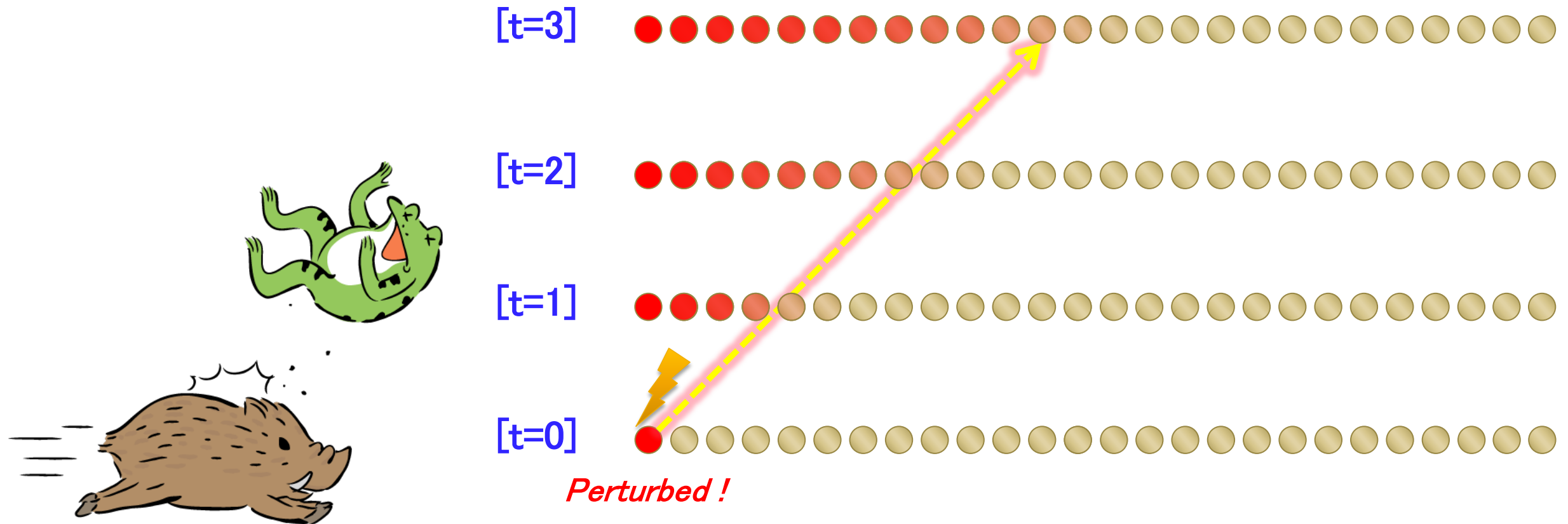
Can we approximate the dynamics with good accuracy by incorporating a “moderate amount” of correlations?

- Rigorous diagonalization: taking all the correlations into account

Solvable only for small systems (~ 20 spins)

Speed limit of information propagation

Perturbation is added to the left-edge spin

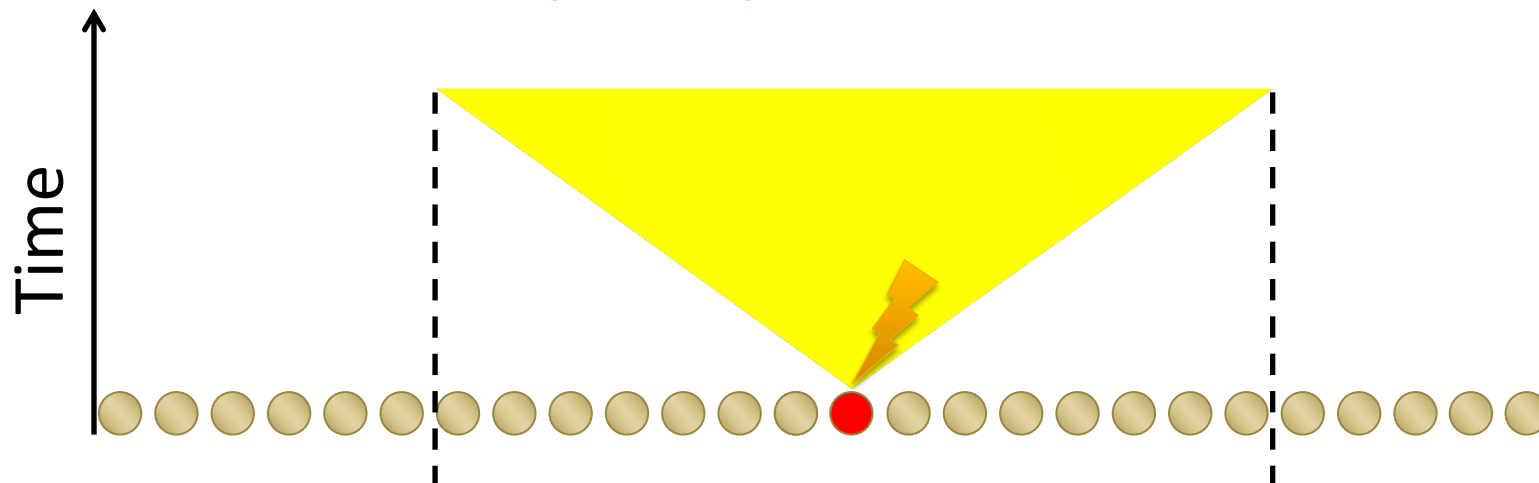


Effective light cone

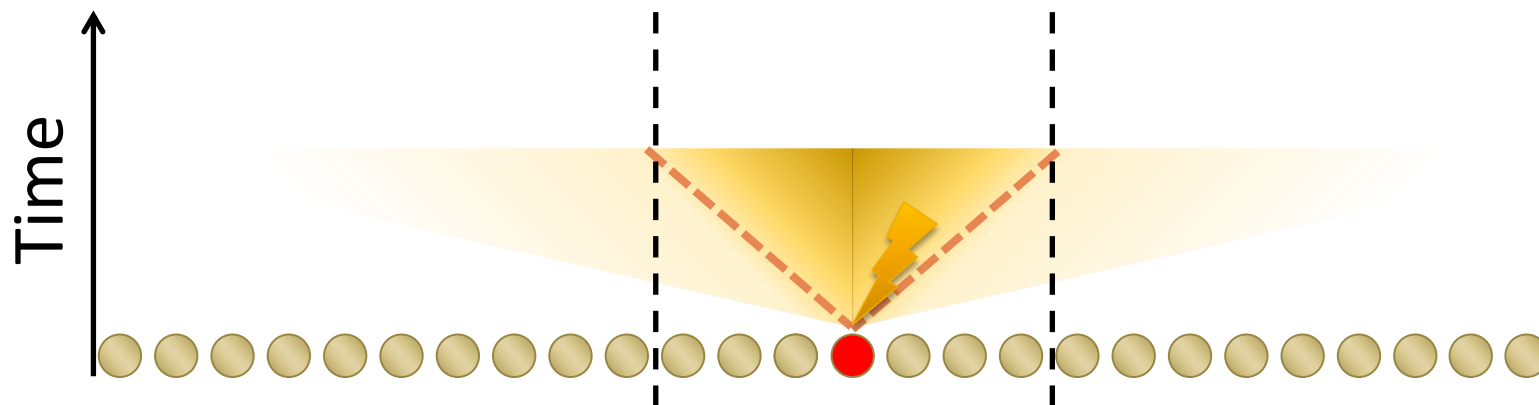


[General limit on the
information propagation]

[Light cone in the relativity theory]



[Effective light cone in the non-relativistic cases]



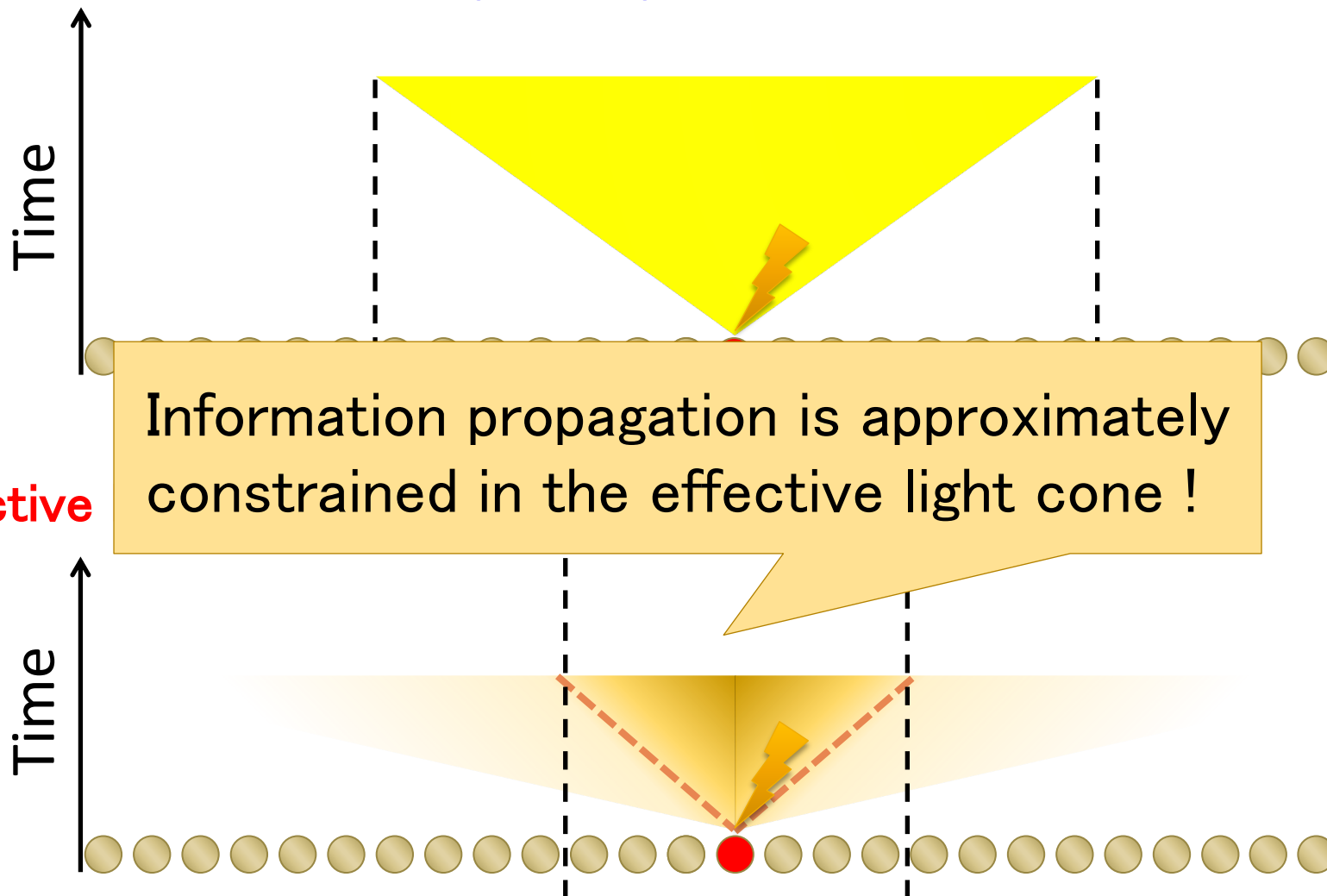
↙
Lieb–Robinson bound

Effective light cone



[Light cone in the relativity theory]

[General limit on the
information propagation]



[Effective

Lieb-Robinson bound

2: Setup

Summary:

Lieb-Robinson bound is formulated by an error bound for the approximation of operator spreading

Operator spreading

- (Basic question)

How fast do local operators spread over time evolution?



Operator spreading

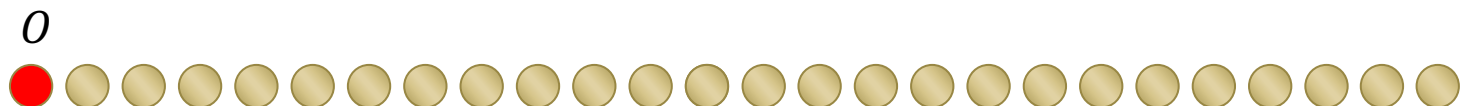
- (Basic question)

How fast do local operators spread over time evolution?

- Time evolution of an arbitrary operator O (Heisenberg picture)

$$O(t) = e^{iHt} O e^{-iHt} = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \overbrace{[H, [H, [H, \dots, [H, O]] \dots]}^n$$

➡ Even if the operator O is local at $t = 0$, the time evolved $O(t)$ is usually non-local !



Specific example

- Hamiltonian: one-dimensional Heisenberg chain

$$H = \sum_{i=1}^{N-1} J(\sigma_i^x \otimes \sigma_{i+1}^x + \sigma_i^y \otimes \sigma_{i+1}^y + \sigma_i^z \otimes \sigma_{i+1}^z)$$

- Let $O = \sigma_1^z$ and consider $O(t) = e^{iHt} \sigma_1^z e^{-iHt}$

$$[H, A] = \underbrace{2iJ(\sigma_1^y \sigma_2^x - \sigma_1^x \sigma_2^y)}$$

Including the spins 1 and 2

0



$$J(\sigma_i^x \otimes \sigma_{i+1}^x + \sigma_i^y \otimes \sigma_{i+1}^y + \sigma_i^z \otimes \sigma_{i+1}^z)$$

$$[H, [H, A]] = \underbrace{4J^2(\sigma_1^x \sigma_2^x \sigma_3^z - \sigma_1^x \sigma_2^z \sigma_3^x + \sigma_1^y \sigma_2^y \sigma_3^z - \sigma_1^y \sigma_2^z \sigma_3^y + 2\sigma_1^z - 2\sigma_2^z)}$$

Including the spins 1, 2 and 3

$$\overbrace{[H, [H, [H, \dots, [H, A]]]}^n : \text{Including the spins } 1, 2, 3, \dots, n$$

Lieb-Robinson bound

- Upper bound on the commutator norm: $\|[O_i(t), O_j]\|$ $\|\cdots\|$: operator norm

- Under two conditions

➔ (1) Interactions are short-range

$$h_{i,j} = 0 \quad \text{for} \quad d_{i,j} \geq \text{const.}$$

➔ (2) One-site energy is finitely bounded

$$\sum_{j \neq i} \|h_{i,j}\| + \|h_i\| = \text{const.} \quad \text{for} \quad \forall i \in \Lambda$$

$d_{i,j}$: distance between i and j

$\|O\|$:= Square root of the maximum eigenvalue of $O^\dagger O$

➔ For $\forall |\psi\rangle$, we have $\langle \psi | O^\dagger O | \psi \rangle \leq \|O\|^2$

$i, j \in \Lambda$ $i=1$

$$1 + \sigma_i^z \otimes \sigma_{i+1}^z$$

[Lieb-Robinson bound]

Lieb and Robinson, Commun. Math. Phys. **28**, 251 (1972).

$$\|[O_i(t), O_j]\| \leq \|O_i\| \cdot \|O_j\| e^{-c(d_{i,j} - vt)}$$

Lieb-Robinson bound

- Upper bound on the commutator norm: $\|[O_i(t), O_j]\|$ $\|\cdots\|$: operator norm

- Under two conditions**

➔ **(1) Interactions are short-range**

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$d_{i,j}$: distance between i and j

$$H = \sum_{i=1}^{N-1} J(\sigma_i^x \otimes \sigma_{i+1}^x + \sigma_i^y \otimes \sigma_{i+1}^y + \sigma_i^z \otimes \sigma_{i+1}^z)$$



generalize

$$H = \sum_{i,j \in \Lambda} h_{i,j} + \sum_{i=1}^n h_i$$

[Lieb-Robinson bound]

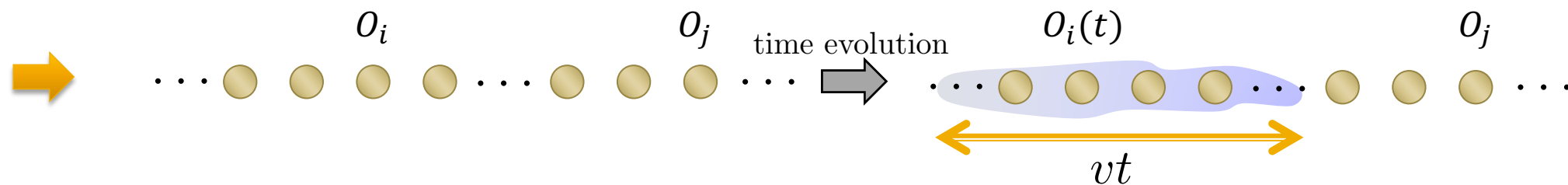
Lieb and Robinson, Commun. Math. Phys. **28**, 251 (1972).

$$\|[O_i(t), O_j]\| \leq \|O_i\| \cdot \|O_j\| e^{-c(d_{i,j} - vt)}$$

Physical meaning

- The operator spreads linearly with time

$$\|[O_i(t), O_j]\| \leq \|O_i\| \cdot \|O_j\| e^{-c(d_{i,j} - vt)}$$



- Contribution beyond $d_{i,j} \gtrsim vt$ decays exponentially with distance
- It means that the speed of information propagation is finite

Why?

Quantum state transfer

■ Quantum state transfer

S. Bravyi, et al., PRL 97, 050401 (2006).

➡ Initial state ρ_0 , e.g., product state of $|0\rangle$ with R qubits

➡ Unitary operation to left-edge spin A, e.g., $u_0 = \hat{1}$ or $u_1 = |1\rangle\langle 0| + |0\rangle\langle 1|$

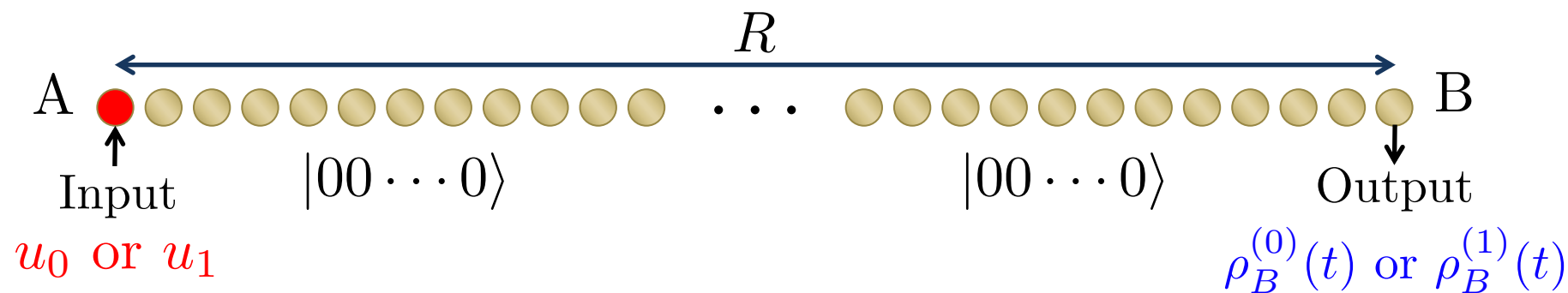
➡ Time evolution $\rho(t) = U_t^\dagger (u_s^\dagger \rho_0 u_s) U_t$ $s = 0$ or 1

$$\rho_B^{(s)}(t) := \text{tr}_{B^c} \left[U_t^\dagger (u_s^\dagger \rho_0 u_s) U_t \right]$$

$$U_t = \mathcal{T} e^{-i \int_0^t H(\tau) d\tau}$$

$H(\tau)$: Time-dependent Hamiltonian

➡ Can we distinguish $\rho_B^{(0)}(t)$ and $\rho_B^{(1)}(t)$?



Quantum state transfer

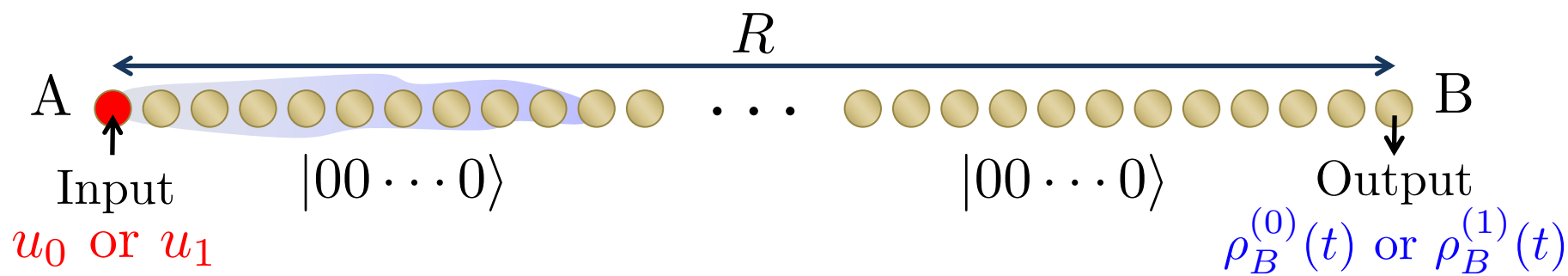
- At $t = 0$, we have $U_t = \hat{1} \longrightarrow \rho_B^{(s)}(0) = \text{tr}_{B^c} (u_s^\dagger \rho_0 u_s) = \text{tr}_{B^c} (\rho_0 u_s u_s^\dagger) = \text{tr}_{B^c} (\rho_0)$

$\longrightarrow$ The same outputs for $s = 0$ and 1 $\|\rho_B^{(1)}(t) - \rho_B^{(0)}(t)\|_1 = 0$

- If $\rho_B^{(1)}(t)$ and $\rho_B^{(0)}(t)$ is orthogonal, i.e., $\|\rho_B^{(1)}(t) - \rho_B^{(0)}(t)\|_1 = 2$, we can achieve perfect state transfer.

- Lieb-Robinson bound gives the upper bound

$$\|\rho_B^{(1)}(t) - \rho_B^{(0)}(t)\|_1 \leq \sup_{O_B: \|O_B\|=1} \|[u_1 u_0^\dagger, O_B(t)]\| \leq e^{-c(R-vt)}$$



Quantum state transfer

- The amount of information transferred from A to B is characterized by $\|\rho_B^{(1)}(t) - \rho_B^{(0)}(t)\|_1$, which decays exponentially as $e^{-c(R-vt)}$!

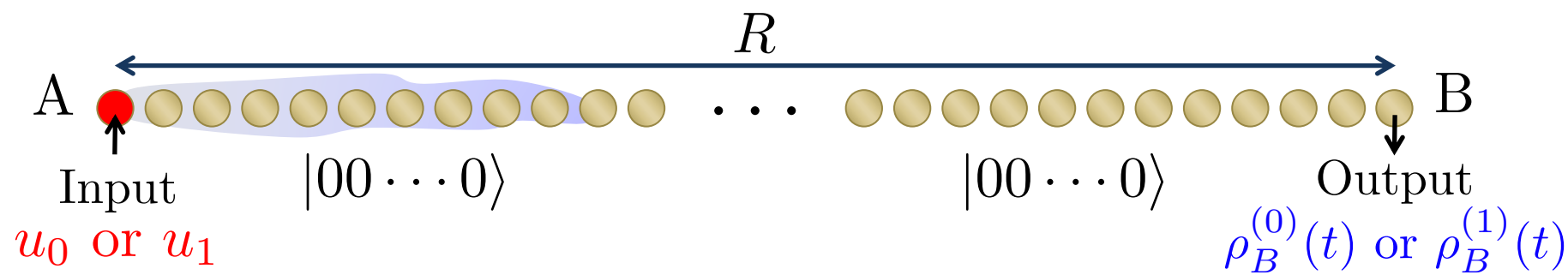
➡ The Holevo capacity characterizes the amount of information transfer more rigorously

$$(\rho_0 u_s u_s^\dagger) = \text{tr}_{B^c}(\rho_0)$$

S. Bravyi, et al., PRL **97**, 050401 (2006).
A. S. Holevo, Probl. Inf. Transm. **9**, 177 (1973).

- Lieb-Robinson bound is the upper bound

$$\|\rho_B^{(1)}(t) - \rho_B^{(0)}(t)\|_1 \leq \sup_{O_B: \|O_B\|=1} \|[u_1 u_0^\dagger, O_B(t)]\| \leq e^{-c(R-vt)}$$



3: Derivation

Summary:

My PhD thesis Sec. 2.7

http://hatano-lab.iis.u-tokyo.ac.jp/thesis/dron2014/thesis_kuwahara.pdf

Applications of Lieb-Robinson bound

Summary:

Clever uses of the Fourier transformation are the keys

Fourier transformation

- Target operator $\hat{O}$

$$e^{-i\omega t} \hat{A}_\omega = e^{iHt} \hat{A}_\omega e^{-iHt}$$

$$\hat{O} = \int_{-\infty}^{\infty} f(\omega) \hat{A}_\omega d\omega, \quad \hat{A}_\omega = \sum_{E, E'} \delta(E' - E - \omega) \langle E | \hat{A} | E' \rangle |E\rangle \langle E'|$$

 **Fourier transformation**

$$\hat{O} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-i\omega t} \tilde{f}(t) dt \hat{A}_\omega d\omega = \int_{-\infty}^{\infty} \tilde{f}(t) \hat{A}(t) dt$$

$$\int_{-\infty}^{\infty} e^{-i\omega t} \hat{A}_\omega d\omega = \hat{A}(t)$$

Exponentially decays in various applications

$$\int_{-\infty}^{\infty} \tilde{f}(t) \hat{A}(t) dt \approx \int_{-\bar{t}}^{\bar{t}} \tilde{f}(t) \hat{A}(t) dt$$

- The point is how to calculate the property of $\tilde{f}(t)$ appropriately

Example. Clustering theorem

- Clustering theorem

$$P_0 = |E_0\rangle\langle E_0|, \quad Q_0 = 1 - P_0$$

Let $|E_0\rangle$ be the ground state of a Hamiltonian H .

Then, for arbitrary two operators O_i and O_j ,

The bi-partite correlation

$$\langle E_0|O_i O_j|E_0\rangle - \langle E_0|O_i|E_0\rangle\langle E_0|O_j|E_0\rangle \quad \leftarrow \text{Target!}$$

decays exponentially as follows:

$$|\langle E_0|O_i O_j|E_0\rangle - \langle E_0|O_i|E_0\rangle\langle E_0|O_j|E_0\rangle| \leq \|O_i\| \cdot \|O_j\| e^{-\text{const} d_{i,j}/\xi},$$

where ξ is the correlation length as $\xi \propto 1/\Delta$ (Δ : spectral gap).

Clustering theorem

■ Clustering theorem

$$P_0 = |E_0\rangle\langle E_0|, \quad Q_0 = 1 - P_0$$

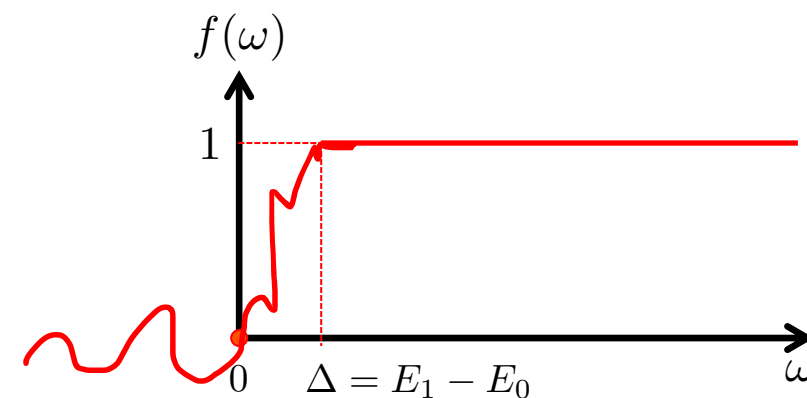
$$\hat{O} = \frac{P_0 O_i Q_0 O_j P_0 + P_0 O_j Q_0 O_i P_0}{2}, \quad \leftarrow \langle E_0 | O_i O_j | E_0 \rangle - \langle E_0 | O_i | E_0 \rangle \langle E_0 | O_j | E_0 \rangle$$

↓ Spectral decomposition

$$\hat{O} = \int_{-\infty}^{\infty} P_0 f(\omega) [(O_i)_\omega O_j + O_j (O_i)_{-\omega}] d\omega P_0,$$

↓ (approximate) Fourier transformation

$$\hat{O} \approx \int_{-\infty}^{\infty} P_0 \tilde{f}(t) [O_i(t) O_j + O_j O_i(-t)] d\omega P_0,$$



$$\tilde{f}(-t) = -\tilde{f}(t)$$

Clustering theorem

■ Clustering theorem

$$P_0 = |E_0\rangle\langle E_0|, \quad Q_0 = 1 - P_0$$

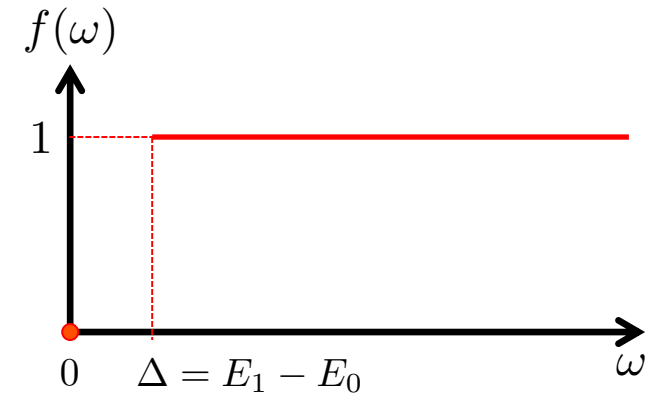
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↓ Spectral decomposition

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Clustering theorem

■ Clustering theorem

$$P_0 = |E_0\rangle\langle E_0|, \quad Q_0 = 1 - P_0$$

$$\hat{O} = \frac{P_0 O_i Q_0 O_j P_0 + P_0 O_j Q_0 O_i P_0}{2}, \quad \leftarrow \langle E_0 | O_i O_j | E_0 \rangle - \langle E_0 | O_i | E_0 \rangle \langle E_0 | O_j | E_0 \rangle$$

Spectral de

$$\hat{O} = \int_{-\infty}^{\infty} P_0 f(\omega) [(O_i(t) O_j - O_j O_i(t))] d\omega P_0,$$

Fourier transform

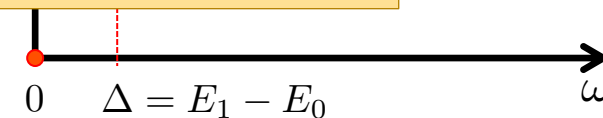
$$\hat{O} \approx \int_{-\infty}^{\infty} P_0 \tilde{f}(t) [O_i(t) O_j - O_j O_i(t)] d\omega P_0,$$

$$\tilde{f}(t) \propto e^{-c(t/\mu)^2} \quad \mu: \text{free parameter}$$

Precision error $\epsilon = e^{-c'(\mu\Delta)^2}$ $\Delta = E_1 - E_0$

$$\|\hat{O}\| \leq e^{-\mathcal{O}(d_{i,j}\Delta)} \quad (\mu \propto d_{i,j})$$

Hastings and Koma, CMP **265**, 781 (2006).



$$\tilde{f}(-t) = -\tilde{f}(t)$$

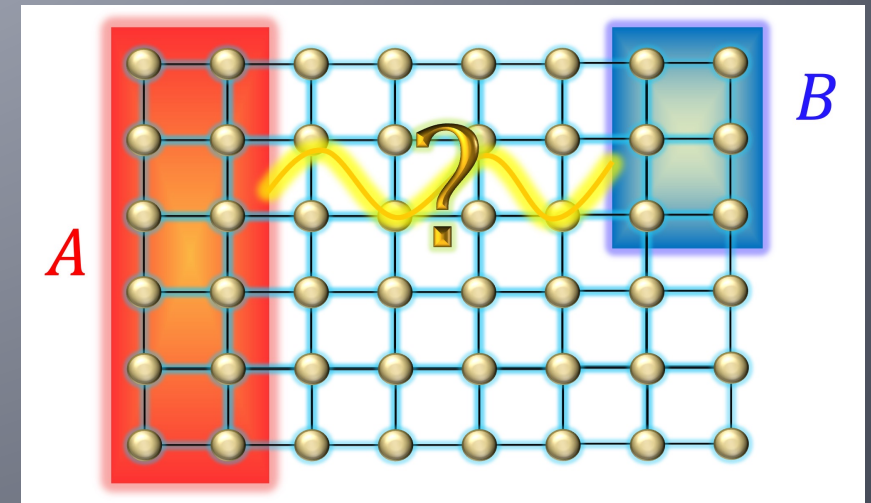
Recent application of the Lieb-Robinson bound

Exponential clustering of bipartite quantum entanglement at arbitrary temperatures

Collaboration with Keiji Saito (Keio U.)

Presented in QIP2022

Physical Review X **12**, 021022 (2022)



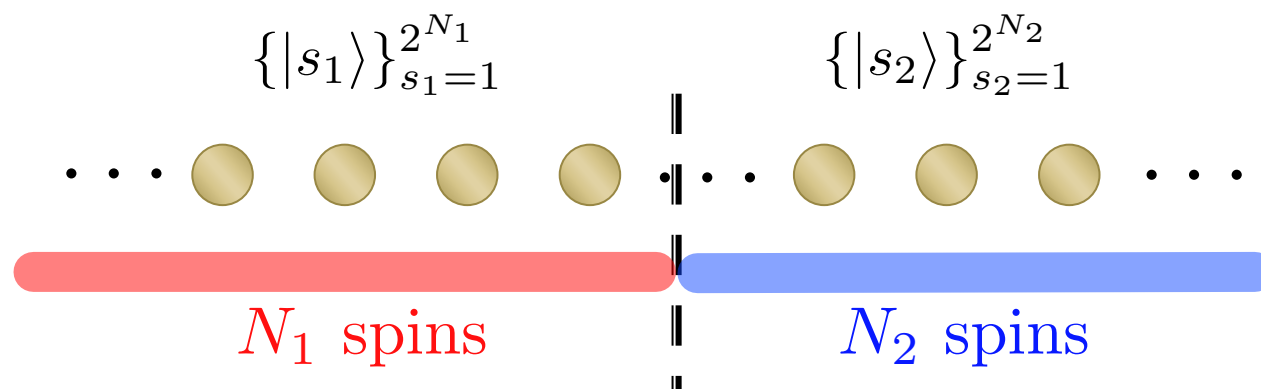
Basics of the quantum entanglement

Entanglement = Quantum correlation that results from the superposition principle

Then, how to define it?

Definition of bipartite entanglement

- One dimensional chain



- General states: $|\psi\rangle = \sum_{s_1=1}^{2^{N_1}} \sum_{s_2=1}^{2^{N_2}} \alpha_{s_1, s_2} |s_1\rangle \otimes |s_2\rangle$

- Zero entanglement $\longleftrightarrow$ Decomposed to product state

$$|\psi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle$$

How to judge?

- Entangled state: e.g., $\frac{1}{\sqrt{2}}(|0, 0\rangle + |1, 1\rangle)$ (Bell state)
- Non-entangled state: e.g., $|0, 0\rangle$
- Then, how about the following two states?

$$\frac{|0, 0\rangle + |0, 1\rangle + |0, 1\rangle + |1, 1\rangle}{2}$$

$$\frac{|0, 0\rangle + |0, 1\rangle + |0, 1\rangle - |1, 1\rangle}{2}$$

How to judge?

- Entangled state: e.g., $\frac{1}{\sqrt{2}}(|0, 0\rangle + |1, 1\rangle)$ (Bell state)
- Non-entangled state: e.g., $|0, 0\rangle$
- Then, how about the following two states?

$$\underbrace{\frac{|0, 0\rangle + |0, 1\rangle + |0, 1\rangle + |1, 1\rangle}{2}}$$

Non entangled

$$\rightarrow \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

$$\underbrace{\frac{|0, 0\rangle + |0, 1\rangle + |0, 1\rangle - |1, 1\rangle}{2}}$$

Entangled

$$\rightarrow \frac{1}{\sqrt{2}} \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |0\rangle + \frac{|0\rangle - |1\rangle}{\sqrt{2}} \otimes |1\rangle \right)$$

Schmidt decomposition

- An arbitrary quantum state can be decomposed as follows:

$$\begin{aligned}
 |\psi\rangle &= \sum_{s_1=1}^{2^{N_1}} \sum_{s_2=1}^{2^{N_2}} \alpha_{s_1, s_2} |s_1\rangle \otimes |s_2\rangle \\
 &= \sum_{s=1}^{2^{N_0}} \lambda_s |\phi_{1s}\rangle \otimes |\phi_{2s}\rangle \quad N_0 = \min(N_1, N_2)
 \end{aligned}$$

$1 \geq \lambda_1 \geq \lambda_2 \geq \dots \lambda_{2^{N_0}} \geq 0$

Orthonormal states for system 1 Orthonormal states for system 2

Schmidt decomposition

- An arbitrary quantum state

$$|\psi\rangle = \sum_{s_1=1}^{2^{N_1}} \sum_s$$

$$= \sum_{s=1}^{2^{N_0}} \lambda_s |\phi_{1s}\rangle \otimes |\phi_{2s}\rangle$$

$$1 \geq \lambda_1 \geq \lambda_2 \geq \dots \lambda_{2^{N_0}} \geq 0$$

Orthonormal states for system 1

Orthonormal states for system 2

If there are no entanglement

$$\lambda_1 = 1, \lambda_2 = \lambda_3 = \dots = \lambda_{2^{N_0}} = 0$$

$$\rightarrow |\psi\rangle = |\phi_{11}\rangle \otimes |\phi_{21}\rangle$$

$$N_0 = \min(N_1, N_2)$$

Schmidt decomposition: derivation 1

- Base conversion for system 1: $U^{(1)}$

$$U^{(1)}|s_1\rangle = \sum_{s'_1} U_{s_1,s'_1}^{(1)}|s'_1\rangle$$

$$\text{e.g., } U^{(1)} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}$$

$$U^{(1)}|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$U^{(1)}|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

- Base conversion for system 2: $U^{(2)}$

$$U^{(2)}|s_2\rangle = \sum_{s'_2} U_{s_2,s'_2}^{(2)}|s'_2\rangle$$

- We want to find appropriate base conversions

Schmidt decomposition: derivation 2

- Base conversions for the systems 1 and 2

$$\begin{aligned}
 U^{(1)} \otimes U^{(2)} |\psi\rangle &= \sum_{s_1=1}^{2^{N_1}} \sum_{s_2=1}^{2^{N_2}} \alpha_{s_1, s_2} U^{(1)} |s_1\rangle \otimes U^{(2)} |s_2\rangle \\
 &= \sum_{s'_1, s'_2} \sum_{s_1, s_2} U^{(1)}_{s_1, s'_1} \alpha_{s_1, s_2} U^{(2)}_{s_2, s'_2} |s'_1\rangle \otimes |s'_2\rangle
 \end{aligned}$$

We can regard it as $2^{N_1} \times 2^{N_2}$ matrix

- Matrix elements $\{\alpha_{s_1, s_2}\}$: converted by matrices $[U^{(1)}]^t$ and $U^{(2)}$

Schmidt decomposition: derivation 3

- $[U^{(1)}]^t$ and $U^{(2)}$: Singular value decomposition for $\{\alpha_{s_1, s_2}\}$

$$\sum_{s_1, s_2} U_{s_1, s'_1}^{(1)} \alpha_{s_1, s_2} U_{s_2, s'_2}^{(2)} = \lambda_{s'_1} \delta_{s'_1, s'_2}, \quad s'_1 \leq 2^{\min(N_1, N_2)}$$



$$\begin{aligned} U^{(1)} \otimes U^{(2)} |\psi\rangle &= \sum_{s'_1, s'_2} \sum_{s_1, s_2} U_{s_1, s'_1}^{(1)} \alpha_{s_1, s_2} U_{s_2, s'_2}^{(2)} |s'_1\rangle \otimes |s'_2\rangle \\ &= \sum_{s'=1}^{2^{\min(N_1, N_2)}} \lambda_{s'} |s'\rangle \otimes |s'\rangle \end{aligned}$$

Schmidt decomposition: derivation 3

- $[U^{(1)}]^t$ and $U^{(2)}$: **Singular value decomposition** for $\{\alpha_{s_1, s_2}\}$

$$\sum_{s_1, s_2} U_{s_1, s'_1}^{(1)} \alpha_{s_1, s_2} U_{s_2, s'_2}^{(2)} =$$

$$U^{(1)} \otimes U^{(2)} |\psi\rangle = \sum_{s'_1, s'_2} \lambda_{s'} |s'_1\rangle \otimes |s'_2\rangle$$

$$2^{\min(N_1, N_2)}$$

$$= \sum_{s'=1} \lambda_{s'} |s'\rangle \otimes |s'\rangle$$

For arbitrary $m \times n$ matrix A , there exists a decomposition as

$$A = U^{(1)} \Lambda U^{(2)}$$

$U^{(1)}$: $m \times m$ unitary matrix

$U^{(2)}$: $n \times n$ unitary matrix

Λ : $m \times n$ diagonal matrix

Schmidt decomposition: derivation 3

- $[U^{(1)}]^t$ and $U^{(2)}$: Singular value decomposition for $\{\alpha_{s_1, s_2}\}$

$$\sum_{s_1, s_2} U_{s_1, s'_1}^{(1)} \alpha_{s_1, s_2} U_{s_2, s'_2}^{(2)} = \lambda_{s'_1} \delta_{s'_1, s'_2}, \quad s'_1 \leq 2^{\min(N_1, N_2)}$$



$$\begin{aligned} U^{(1)} \otimes U^{(2)} |\psi\rangle &= \sum_{s'_1, s'_2} \sum_{s_1, s_2} U_{s_1, s'_1}^{(1)} \alpha_{s_1, s_2} U_{s_2, s'_2}^{(2)} |s'_1\rangle \otimes |s'_2\rangle \\ &= \sum_{s'=1}^{2^{\min(N_1, N_2)}} \lambda_{s'} |s'\rangle \otimes |s'\rangle \end{aligned}$$

Schmidt decomposition: derivation 4

- $[U^{(1)}]^t$ and $U^{(2)}$: Singular value decomposition for $\{\alpha_{s_1, s_2}\}$

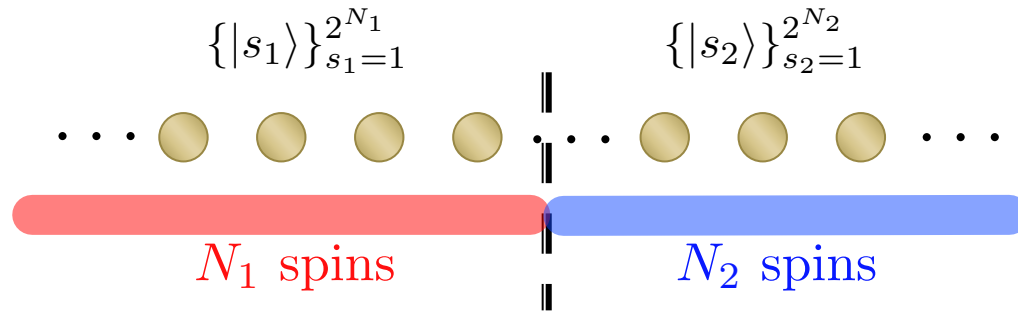
$$U^{(1)} \otimes U^{(2)} |\psi\rangle = \sum_{s'_1, s'_2} \sum_{s_1, s_2} U_{s_1, s'_1}^{(1)} \alpha_{s_1, s_2} U_{s_2, s'_2}^{(2)} |s'_1\rangle \otimes |s'_2\rangle$$

$$= \sum_{s'=1}^{2^{\min(N_1, N_2)}} \lambda_{s'} |s'\rangle \otimes |s'\rangle$$

$$\Rightarrow |\psi\rangle = \sum_{s'=1}^{2^{\min(N_1, N_2)}} \lambda_{s'} U^{(1)\dagger} |s'\rangle \otimes U^{(2)\dagger} |s'\rangle \equiv \sum_{s=1}^{2^{N_0}} \lambda_s |\phi_{1s}\rangle \otimes |\phi_{2s}\rangle$$

Entanglement entropy

- Schmidt decomposition: $|\psi\rangle = \sum_{s=1}^{2^{N_0}} \lambda_s |\phi_{1s}\rangle \otimes |\phi_{2s}\rangle$ $N_0 = \min(N_1, N_2)$



$$E(\psi) := - \sum_s \lambda_s^2 \log \lambda_s^2$$

Zero entanglement

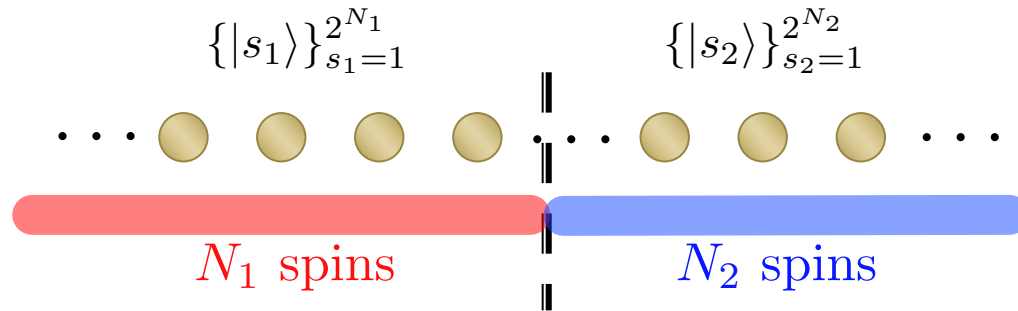
$$\lambda_1 = 1, \lambda_2 = \lambda_3 = \dots = \lambda_{2^{N_0}} = 0 \rightarrow S(\psi) = 0$$

Maximally entangled

$$\lambda_1 = \lambda_2 = \lambda_3 = \dots = \lambda_{2^{N_0}} = 2^{-N_0/2} \rightarrow S(\psi) = N_0$$

Entanglement entropy

- Schmidt decomposition: $|\psi\rangle = \sum_{s=1}^{2^{N_0}} \lambda_s |\phi_{1s}\rangle \otimes |\phi_{2s}\rangle$ $N_0 = \min(N_1, N_2)$



$$E(\psi) := - \sum_s \lambda_s^2 \log \lambda_s^2$$

Zero entanglement

$$\lambda_1 = 1, \lambda_2 = \dots = 0$$

Maximally entangled

$$\lambda_1 = \lambda_2 = \lambda_3 = \dots = \lambda_{2^{N_0}} = 2^{-N_0/2} \rightarrow E(\psi) = N_0$$

Measure of quantum correlation!

Entanglement in mixed state

- Any mixed state $\rho \rightarrow$ infinite patterns of decompositions

$$\rho = \sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j| = \sum_j p_j |\phi_j\rangle\langle\phi_j| \longrightarrow \rho = \sum_j \sqrt{p_j} |\psi_j\rangle\langle\psi_j| \sqrt{p_j} \quad \{\psi_j\} : \text{arbitrary orthonormal bases}$$

$$\sum_j |\psi_j\rangle\langle\psi_j| = \hat{1}$$

- Quantum entanglement in mixed states

ρ is not entangled $\longleftrightarrow$ There exists a decomposition such that all the decomposed states are product states

Entanglement of formation

$$E_F(\rho) := \inf_{\{p_j, \phi_j\}} \sum_j p_j E(\phi_j)$$

- No established method to analyze the entanglement in mixed states...

Motivation

Summary:

Characterization of long-range entanglement at non-zero temperatures

Macroscopic quantum entanglement

- Macroscopic quantum effect at non-zero temperatures

Superconductivity, superfluidity, Bose-Einstein condensation

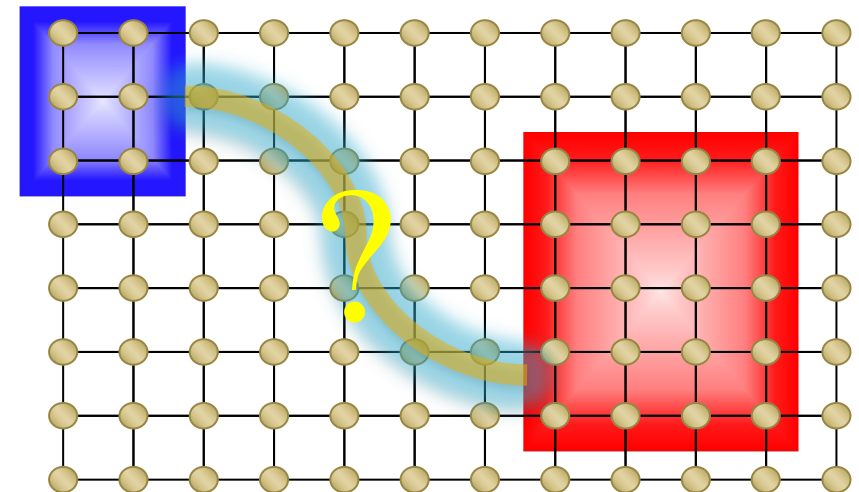


- Macroscopic entanglement at non-zero temperatures

Entanglement is fragile to thermal noise

- Long-range entanglement
- Macroscopic superposition

→ Q. Can the macroscopic entanglement exist at room temperature?



Macroscopic quantum entanglement

- **Macroscopic quantum effect** at non-zero temperatures

Superconductivity, superfluidity, Bose-Einstein condensation



- **Macroscopic entanglement**

Entanglement is **fragile** to

- **Long-range entanglement**
- **Macroscopic entanglement**

The answer is yes, for long-range entanglement

4D: exists in Toric code model

M. B. Hastings, PRL **107**, 210501 (2011)

3D: Controversial

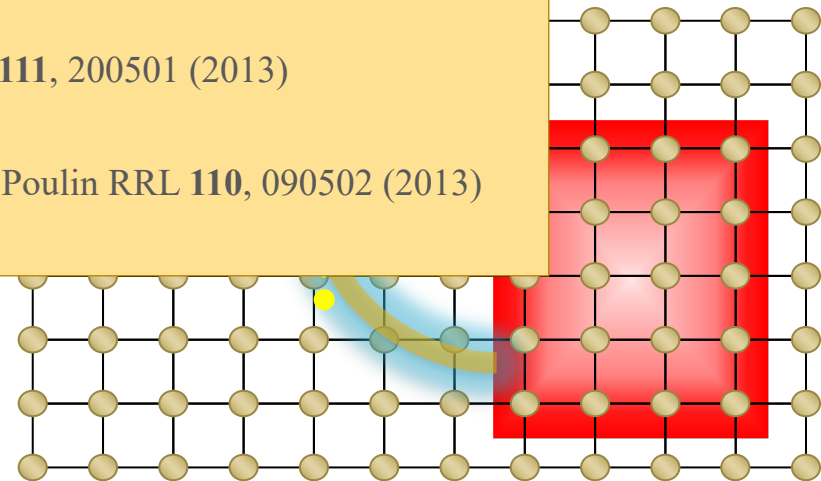
S. Bravyi and J. Haah RRL **111**, 200501 (2013)

1D-2D: probably no.

O. Landon-Cardinal and D. Poulin RRL **110**, 090502 (2013)

A. Lucia, et al., TQC2021.

→ **Q. Can the macroscopic entanglement exist at room temperature?**



Form of long-range entanglement

- A known example in 4D Toric code

M. B. Hastings, PRL **107**, 210501 (2011)

➡ Long-range entanglement exists **as a topological order**

➡ Topological order is inherently a **tripartite correlation**

Kitaev and Preskill, PRL **96**, 110404 (2006)
Levin and Wen, PRL **96**, 110405 (2006)

K. Kato, F. Furrer, and M. Murao, PRA **93**, 022317 (2016).

➡ **Mathematically rigorous that long-range entanglement only exists as (more than) tri-partite correlations?**

[Conjecture]

In arbitrary quantum many-body systems at non-zero temperatures, bi-partite entanglement necessarily decays to zero with the distance.

Set up and obtained results

Summary:

Our study clarified certain aspects of quantum entanglement at arbitrary temperatures

Set up: quantum Gibbs states

- Many-body Hamiltonian (n particles, Spatial dimension: D)

$$H = \sum_{i,j \in \Lambda} h_{i,j} + \sum_{i=1}^n h_i \quad \Lambda: \text{total system}$$

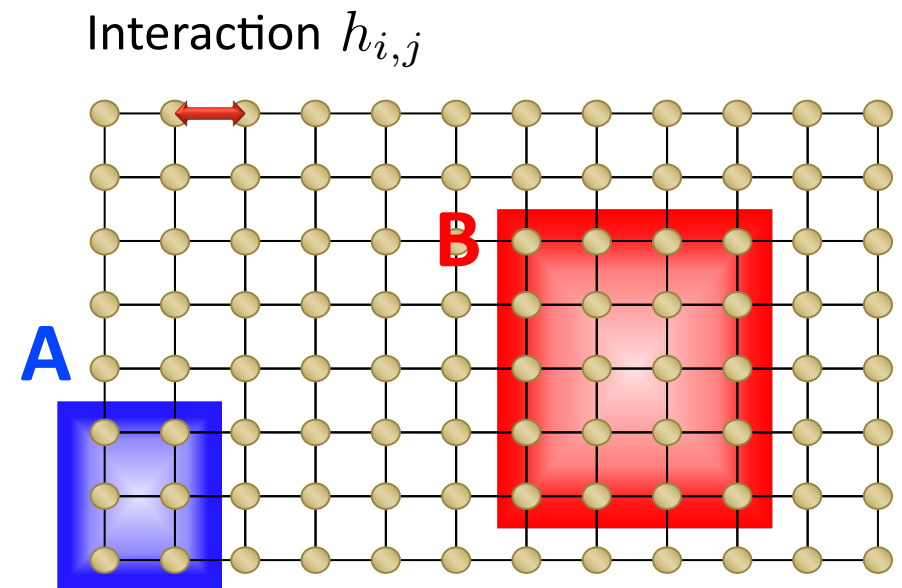
➡ Generalized to arbitrary k -body interactions including long-range interactions

- Quantum Gibbs state

$$\rho_\beta = \frac{e^{-\beta H}}{Z}, \quad Z := \text{tr}(e^{-\beta H})$$

- Reduced density matrix, $A \cup B$

$$\rho_{\beta,AB} = \text{tr}_C(\rho_\beta), \quad C = \Lambda \setminus (AB)$$



Entanglement measure

- Entanglement measures: **Relative entanglement entropy**

V. Vedral et al., Phys. Rev. Lett. **78**, 2275 (1997)

$$E_R(\rho) := \inf_{\sigma \in \text{SEP}} S(\rho || \sigma)$$

Set of non-entangled matrix = SEP


 $\inf_{\sigma \in \text{SEP}} \|\rho - \sigma\|_1 \leq \sqrt{2E_R(\rho)}$

 Other entanglement measure
 (e.g., entanglement of formation)

Pinsker's ineq.

- PPT relative entanglement:**

$$E_R^{\text{PPT}}(\rho) := \inf_{\sigma \in \text{PPT}} S(\rho || \sigma)$$

Set of matrices ρ s.t. $\rho^{T_1} \geq 0$: **PPT (Positive partial transpose)**

K. Audenaert et al., Phys. Rev. Lett. **87**, 217902 (2001)

- $E_R^{\text{PPT}}(\rho) \leq E_R(\rho)$

Mathematical formulation of the conjecture

- Reduced density matrix on $A \cup B$

$$\rho_\beta = \frac{e^{-\beta H}}{Z}, \quad Z := \text{tr}(e^{-\beta H})$$

$$\rho_{\beta, AB} = \text{tr}_C(\rho_\beta), \quad C = \Lambda \setminus (AB)$$

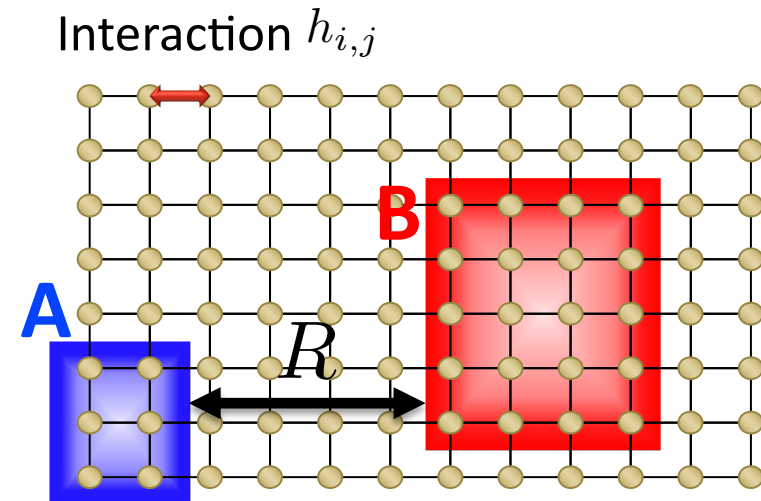
- [Conjecture]

For arbitrary Hamiltonian, the entanglement between A and B decays exponentially with the distance:

$$E_R(\rho_{\beta, AB}) \leq \text{Poly}(|A|, |B|) e^{-R/\xi_\beta} \quad \xi_\beta = \text{Poly}(\beta)$$

- [Weaker conjecture]

$$E_R^{PPT}(\rho_{\beta, AB}) \leq \text{Poly}(|A|, |B|) e^{-R/\xi_\beta} \quad \xi_\beta = \text{Poly}(\beta)$$



Previous works

(β : inverse temperature)

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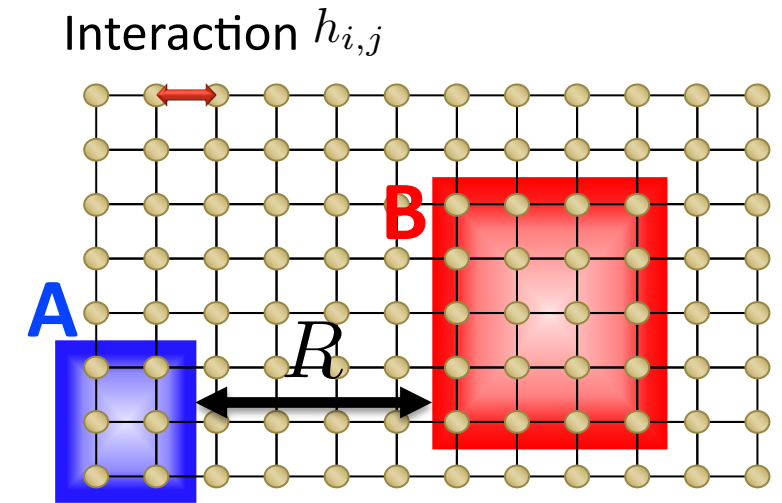
- High-temperature: $\beta < \beta_c$

[Exponential decay of operator correlation]

$$\langle O_A O_B \rangle_{\rho_\beta} - \langle O_A \rangle_{\rho_\beta} \langle O_B \rangle_{\rho_\beta} \leq \min(|A|, |B|) e^{-R/\xi_\beta}$$

$$\langle O \rangle_{\rho_\beta} = \text{tr}(\rho_\beta O), \quad \xi_\beta = O(1)$$

M. Kliesch, et al., PRX (2014). Fröhlich, et al., J. Math. Phys. (2015).



[Exponential decay of mutual information] [Kuwahara, Kato and Brandao, RRL \(2020\)](#)

$$\longrightarrow \|\rho_{\beta,AB} - \rho_{\beta,A} \otimes \rho_{\beta,B}\| \leq \min(|A|, |B|) e^{-R/\xi_\beta}$$

→ **Exponential decay of quantum entanglement**

1D case, better results

Bluhm, Capel and Hernández, QIP 2022, $\xi_\beta = e^{O(\beta)}$ for $\forall \beta$

Previous works

(β : inverse temperature)

67

- High-temperature: $\beta < \beta_c$

[Exponential decay of operator correlation]

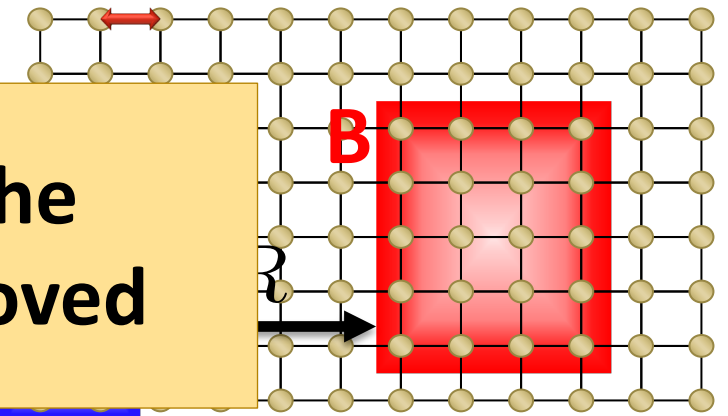
$$\langle O_A O_B \rangle_{\rho_\beta} - \langle O_A \rangle_{\rho_\beta} \langle O_B \rangle_{\rho_\beta} \leq \min(|A|, |B|) e^{-\xi_\beta R}$$

$$\langle O \rangle_{\rho_\beta} = \text{tr}(\rho_\beta O), \quad \xi_\beta = 0(1)$$

M. Kliesch, et al., PRX (2014). Fröhlich, et al.

At high temperatures, the conjecture has been proved

Interaction $h_{i,j}$



[Exponential decay of mutual information]

Kuwahara, Kato and Brandao, RRL (2020)

$$\|\rho_{\beta,AB} - \rho_{\beta,A} \otimes \rho_{\beta,B}\| \leq \min(|A|, |B|) e^{-R/\xi_\beta}$$

Exponential decay of quantum entanglement

1D case, better results

Bluhm, Capel and Hernández, QIP 2022, $\xi_\beta = e^{O(\beta)}$ for $\forall \beta$

Low-temperatures

(β : inverse temperature)

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- Low-temperature: $\beta \geq \beta_c$
→ Phase transition can occur
- Clustering of correlations no longer holds
- There still exists strong restrictions

[Thermal area law]

M. M. Wolf et al., Phys. Rev. Lett. **100**, 070502 (2008).

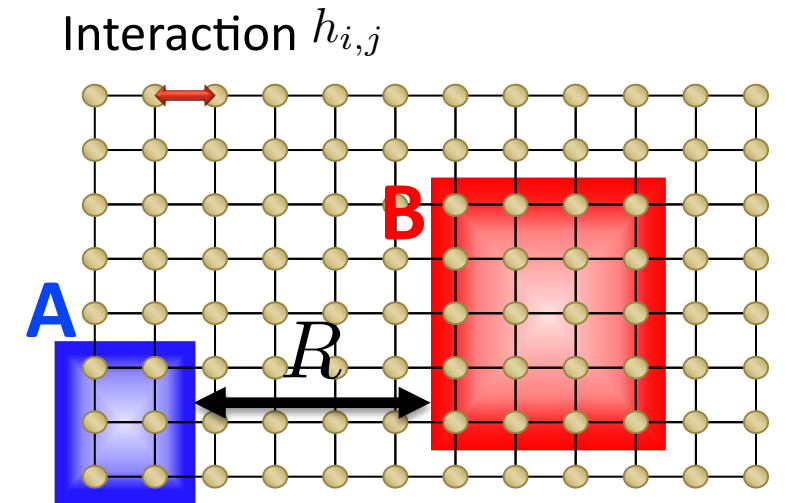
Kuwahara, Alhambra, and Anshu, Phys. Rev. X **11**, 011047 (2021), QIP2021

[Belief propagation]

M. B. Hastings, Phys. Rev. B **76**, 201102 (2007).

→ It is highly non-trivial on what kinds of non-locality are strictly prohibited

- Can we still prove the clustering of quantum entanglement?



Main results on $E_R^{PPT}(\rho_{AB})$

- Reduced density matrix, $A \cup B$

$$\rho_\beta = \frac{e^{-\beta H}}{Z}, \quad Z := \text{tr}(e^{-\beta H})$$

$$\rho_{\beta,AB} = \text{tr}_C(\rho_\beta), \quad C = \Lambda \setminus (AB)$$

- [Theorem, for 1D]

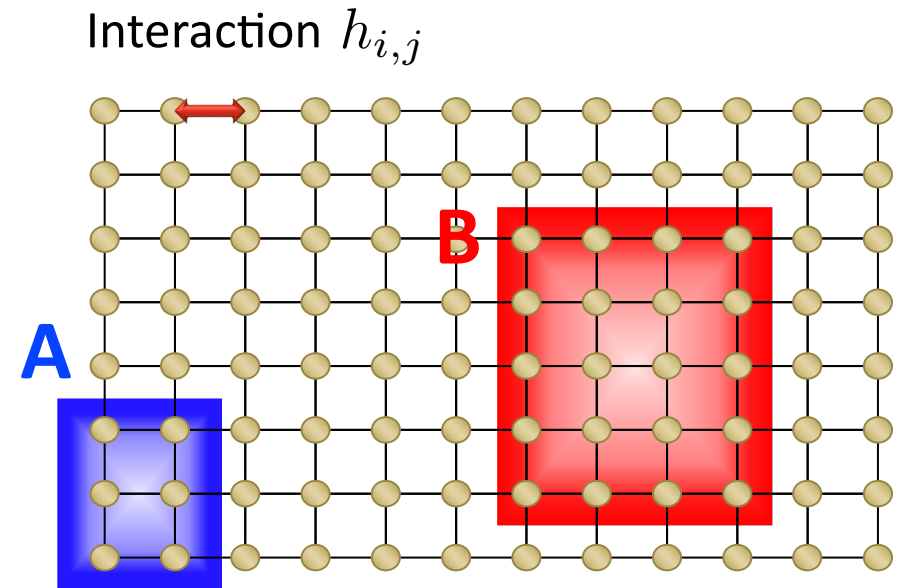
$$E_R^{PPT}(\rho_{\beta,AB}) \leq (|A| + |B|)e^{-R/\xi_\beta}$$

$$\xi_\beta = O(\beta^2)$$

- [Theorem, for 2D-]

$$E_R^{PPT}(\rho_{\beta,AB}) \leq e^{O(|A|+|B|)}e^{-R/\xi_\beta}$$

$$\xi_\beta = O(\beta)$$



Main results on $E_R^{PPT}(\rho_{AB})$

- Reduced density matrix. $A \cup B$

$$\rho_\beta = \frac{e^{-\beta H}}{Z}$$

Can we improve it to $E_R(\rho_{AB})$?

- [Theorem, for 1D]

$$E_R^{PPT}(\rho_{\beta,AB}) \leq (|A| + |B|)e^{-R/\xi_\beta}$$

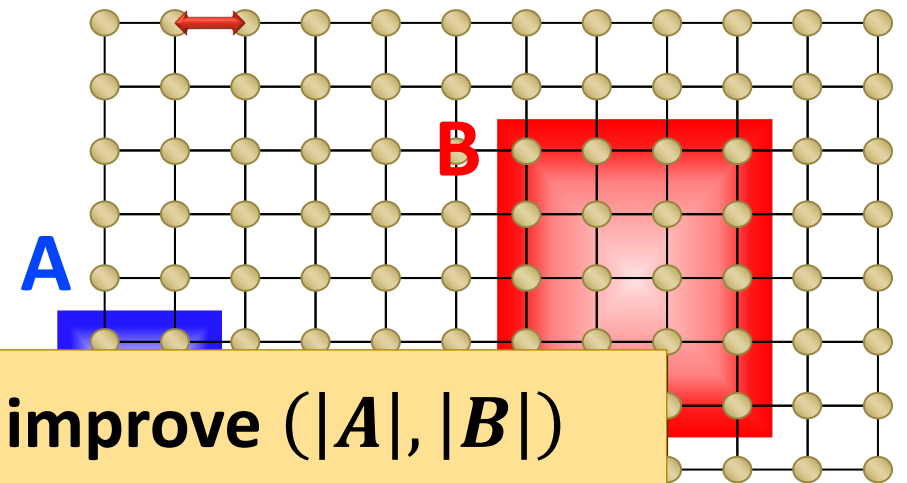
$$\xi_\beta = O(\beta^2)$$

- [Theorem, for 2D-]

$$E_R^{PPT}(\rho_{\beta,AB}) \leq e^{O(|A|+|B|)}e^{-R/\xi_\beta}$$

$$\xi_\beta = O(\beta)$$

Interaction $h_{i,j}$



Can we improve $(|A|, |B|)$ dependence to polynomial form?

Main idea: Quantum correlations

- Convex roof of standard correlations

$$QC_\rho(O_A, O_B) := \inf_{\{p_i, \rho_i\}} \sum_i p_i |C_{\rho_i}(O_A, O_B)| \quad \rho = \sum_i p_i \rho_i$$

$$C_\rho(O_A, O_B) := \langle O_A O_B \rangle_\rho - \langle O_A \rangle_\rho \langle O_B \rangle_\rho$$

Main idea: Quantum correlations

- Convex roof of standard correlations

$$QC_{\rho}(O_A, O_B) := \inf_{\{p_i, \rho_i\}} \sum_i p_i |C_{\rho_i}(O_A, O_B)| \quad \rho = \sum_i p_i \rho_i$$

$$C_{\rho}(O_A, O_B) := \langle O_A O_B \rangle_{\rho} - \langle O_A \rangle_{\rho} \langle O_B \rangle_{\rho}$$

- Relation to Entanglement of formation

$$E_F(\rho_{AB}) := \inf_{\{p_i, \rho_i\}} \sum_i 2p_i I_{\rho_i}(A: B)$$



$$I_{\rho_i}(A: B) \geq \frac{|C_{\rho_i}(O_A, O_B)|^2}{2 \|O_A\|^2 \cdot \|O_B\|^2}$$

$$QC_{\rho_{AB}}(O_A, O_B) \leq 2 \|O_A\| \cdot \|O_B\| \sqrt{E_F(\rho_{AB})}$$

Main idea: Quantum correlations

- Convex roof of standard correlations

$$QC_{\rho}(O_A, O_B) := \inf_{\{p_i, \rho_i\}} \sum_i p_i |C_{\rho_i}(O_A, O_B)| \quad \rho = \sum_i p_i \rho_i$$

$$C_{\rho}(O_A, O_B) := \langle O_A O_B \rangle_{\rho} - \langle O_A \rangle_{\rho} \langle O_B \rangle_{\rho}$$

- ρ_{AB} is not entangled $\rightarrow QC_{\rho_{AB}}(O_A, O_B) = 0$ for $\forall O_A, O_B$

$$\rho_{AB} = \sum_i p_i \rho_{i,AB} \quad \text{s.t.} \quad \rho_{i,AB} = \rho_{i,A} \otimes \rho_{i,B}$$

- [Conjecture] the converse is true.

$$QC_{\rho_{AB}}(O_A, O_B) = 0 \text{ for arbitrary pairs of } O_A, O_B \xrightarrow{?} \rho_{AB} \text{ is not entangled.}$$

$$(\rho_{AB} \in \text{SEP})$$

- We can at least prove

$$QC_{\rho_{AB}}(O_A, O_B) = 0 \text{ for arbitrary pairs of } O_A, O_B \rightarrow \rho_{AB} \in \text{PPT.}$$

Main idea: Quantum correlations

- Convex roof of standard correlations

$$QC_{\rho}(O_A, O_B) := \inf_{\{p_i, \rho_i\}} \sum_i p_i |C_{\rho_i}(O_A, O_B)| \quad \rho = \sum_i p_i \rho_i$$

$$C_{\rho}(O_A, O_B) := \langle O_A O_B \rangle_{\rho} - \langle O_A \rangle_{\rho} \langle O_B \rangle_{\rho}$$

- ρ_{AB} is not entangled $\rightarrow QC_{\rho_{AB}}(O_A, O_B) = 0$ for $\forall O_A, O_B$

$$\rho_{AB} = \sum_i p_i \rho_{i,AB} \quad \text{s.t.} \quad \rho_{i,AB} = \rho_{i,A} \otimes \rho_{i,B}$$

- [Conjecture] the converse

$$QC_{\rho_{AB}}(O_A, O_B) = 0 \text{ for arbitrary pairs } O_A, O_B$$

**Quantum correlation is
connected to PPT condition!**

- We can at least prove

$$QC_{\rho_{AB}}(O_A, O_B) = 0 \text{ for arbitrary pairs of } O_A, O_B \rightarrow \rho_{AB} \in \text{PPT}.$$

Main idea: Exponential decay of quantum correlations

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■ [Theorem]

For arbitrary Hamiltonian and arbitrary temperatures, the entanglement between A and B decays exponentially with the distance:

$$QC_{\rho_{\beta,AB}}(O_A, O_B) = \tilde{O}(|A| + |B|) e^{-R/\xi_\beta}$$

$$\xi_\beta = O(\beta)$$

Lieb-Robinson bound is a key tool

➡ Natural extension of the clustering theorem at high temperatures

■ From the above theorem, we can say

$$QC_{\rho_{\beta,AB}}(O_A, O_B) \approx 0 \text{ for } R \gg 1 \xrightarrow{\quad} \inf_{\sigma_{AB} \in PPT} \|\rho_{\beta,AB} - \sigma_{AB}\|_1 \approx 0$$

$QC_{\rho_{AB}}(O_A, O_B) = 0$
 $\rightarrow \rho_{AB} \in PPT$

$$\downarrow$$
$$E_R^{PPT}(\rho_{\beta,AB}) = \inf_{\sigma_{AB} \in PPT} S(\rho_{\beta,AB} | \sigma_{AB})$$
$$\downarrow$$

Main theorem

Main idea: Exponential decay of quantum correlations

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■ [Theorem]

For arbitrary
between A and B

$$QC_{\rho_{\beta,AB}}(O_A, O_B)$$

→ Natural

■ From the above

If we can achieve the improvement as

$$QC_{\rho_{AB}}(O_A, O_B) = 0 \rightarrow \rho_{AB} \in SEP$$

we will be able to prove

$$\inf_{\sigma_{AB} \in SEP} \|\rho_{\beta,AB} - \sigma_{AB}\|_1 \approx 0$$

on bound is a key tool

$$QC_{\rho_{\beta,AB}}(O_A, O_B) \approx 0 \text{ for } R \gg 1 \quad \longrightarrow \quad \inf_{\sigma_{AB} \in PPT} \|\rho_{\beta,AB} - \sigma_{AB}\|_1 \approx 0$$

$$QC_{\rho_{AB}}(O_A, O_B) = 0 \\ \rightarrow \rho_{AB} \in PPT$$

$$E_R^{PPT}(\rho_{\beta,AB}) = \inf_{\sigma_{AB} \in PPT} S(\rho_{\beta,AB} | \sigma_{AB})$$

Main theorem

Other relevant quantities

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■ Another quantum correlation

Malpetti and Roscilde, PRL 117, 130401 (2016).
Frerot and Roscilde, Nature Commun., 10, 577 (2019).

$$QC_{\rho}^{(\alpha)}(O_A, O_B) := \text{tr}(\rho O_A O_B) - \text{tr}(\rho^{1-\alpha} O_A \rho^{\alpha} O_B) \quad (0 < \alpha < 1)$$


Clustering theorem

$$QC_{\rho_{\beta}}^{(\alpha)}(O_A, O_B) \leq \min(|\partial A|, |\partial B|) e^{-R/\xi_{\beta}}$$

$$\xi_{\beta} = O(\beta)$$

■ Relation to macroscopic superposition

[Wigner–Yanase–Dyson skew information]

$$I_{\rho}^{(\alpha)}(K) := \text{tr}(\rho K^2) - \text{tr}(\rho^{1-\alpha} K \rho^{\alpha} K), \quad K = \sum_{i \in \Lambda} O_i$$



Clustering theorem

$$I_{\rho_{\beta}}^{(\alpha)}(K) \leq O(\xi_{\beta}^D) n = O(\beta^D) n$$

$$I_{\rho}^{(\alpha)}(K) = \sum_{i,j} QC_{\rho_{\beta}}^{(\alpha)}(O_i, O_j)$$

Other relevant quantities

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- Relation to **macroscopic superposition**

[Wigner–Yanase–Dyson skew information]

$$I_{\rho}^{(\alpha)}(K) := \text{tr}(\rho K^2) - \text{tr}(\rho^{1-\alpha} K \rho^{\alpha} K), \quad K = \sum_{i \in \Lambda} O_i$$

$$I_{\rho_{\beta}}^{(\alpha)}(K) \leq O(\xi_{\beta}^D) n = O(\beta^D) n$$

[Quantum Fisher information]

$$\mathcal{F}_{\rho}(K) := \sum_{j,j'} \frac{2(\lambda_j - \lambda_{j'})^2}{\lambda_j + \lambda_{j'}} |\langle \lambda_j | K | \lambda_{j'} \rangle|^2, \quad \rho = \sum_j \lambda_j |\lambda_j\rangle \langle \lambda_j|$$



$$\mathcal{F}_{\rho}(K) \leq 2I_{\rho}^{(1/2)}(K)$$

S. Luo, Proc. Am. Math. Soc. **132**, 885–890 (2004).

$$\mathcal{F}_{\rho_{\beta}}(K) \leq O(\beta^D) n$$

(n : system size)

Other relevant quantities

79

■ Relation to **macroscopic superposition**

[Wigner–Yanase–Dyson skew information]

$$I_{\rho}^{(\alpha)}(K) := \text{tr}(\rho K^2) - \text{tr}(\rho^{1-\alpha} K \rho^{\alpha} K), \quad K = \sum_{i \in \Lambda} O_i$$

$$I_{\rho_{\beta}}^{(\alpha)}(K) \leq O(\xi_{\beta}^D)$$

Quantum Fisher information is a measure for macroscopic superposition

Frowis and Dür, New Journal of Physics **14**, 093039 (2012)

[Quantum Fisher info]

$$\mathcal{F}_{\rho}(K) := \sum_{j,j'} \frac{2(\lambda_j - \lambda_{j'})^2}{\lambda_j + \lambda_{j'}} |\langle j | K | j' \rangle|^2$$

As long as $\beta = \text{Polylog}(n)$, there are no macroscopic superposition in quantum Gibbs states



$$\mathcal{F}_{\rho}(K) \leq 2I_{\rho}^{(1/2)}(K)$$

S. Luo, Proc. Am. Math. Soc. **132**, 885–890 (2004).

$$\mathcal{F}_{\rho_{\beta}}(K) \leq O(\beta^D) n$$

(n : system size)

Proof technique: Clustering of quantum correlation

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- $QC_{\rho}^{(\alpha)}(O_A, O_B) := \text{tr}(\rho O_A O_B) - \text{tr}(\rho^{1-\alpha} O_A \rho^{\alpha} O_B) \quad (0 < \alpha < 1)$

→ $QC_{\rho_{\beta}}^{(\alpha)}(O_A, O_B) = \int_{-\infty}^{\infty} g_{\alpha, \beta}(t) \text{tr}(\rho_{\beta} [O_A(t), O_B]) dt$

Fourier transform technique

$$g_{\alpha, \beta}(t) = -i\beta^{-1} \sum_{m=1}^{\infty} \text{sign}(t) e^{-\frac{2\pi m|t|}{\beta}} (-1 + e^{-2\pi i \alpha m \text{sign}(t)}) \quad (0 < \alpha < 1)$$

$$\left(|g_{\alpha, \beta}(t)| \leq 2\beta^{-1} \frac{e^{-2\pi m|t|/\beta}}{1 - e^{-2\pi m|t|/\beta}} \right)$$



$$QC_{\rho_{\beta}}^{(\alpha)}(O_A, O_B) \leq \min(|\partial A|, |\partial B|) e^{-R/\xi_{\beta}}$$

Lieb-Robinson bound

$$\xi_{\beta} = O(\beta)$$

- Conjecture on the bi-partite entanglement:

$$E_R(\rho_{\beta,AB}) \leq \text{Poly}(|A|, |B|) e^{-R/\xi_\beta} \quad \xi_\beta = \text{Poly}(\beta)$$

- We prove a weaker statement

$$1D : E_R^{PPT}(\rho_{\beta,AB}) \leq (|A| + |B|) e^{-R/\xi_\beta} \\ \xi_\beta = O(\beta^2)$$

$$2D-: E_R^{PPT}(\rho_{\beta,AB}) \leq e^{O(|A|+|B|)} e^{-R/\xi_\beta} \\ \xi_\beta = O(\beta)$$



$$QC_\rho(O_A, O_B) := \inf_{\{p_i, \rho_i\}} \sum_i p_i |C_{\rho_i}(O_A, O_B)|$$

$$QC_{\rho_{\beta,AB}}(O_A, O_B) = \tilde{O}(|A| + |B|) e^{-R/\xi_\beta} \quad \xi_\beta = O(\beta)$$

- Wigner–Yanase–Dyson skew information, Quantum Fisher information

$$I_{\rho_\beta}^{(\alpha)}(K) \leq O(\beta^D) n, \quad \mathcal{F}_{\rho_\beta}(K) \leq O(\beta^D) n \quad \longleftarrow \quad \text{tr}(\rho O_A O_B) - \text{tr}(\rho^{1-\alpha} O_A \rho^\alpha O_B) \leq \min(|\partial A|, |\partial B|) e^{-R/\xi_\beta}$$

Recent progress for Bosonic Lieb-Robinson bound

Two condition for the Lieb-Robinson bound

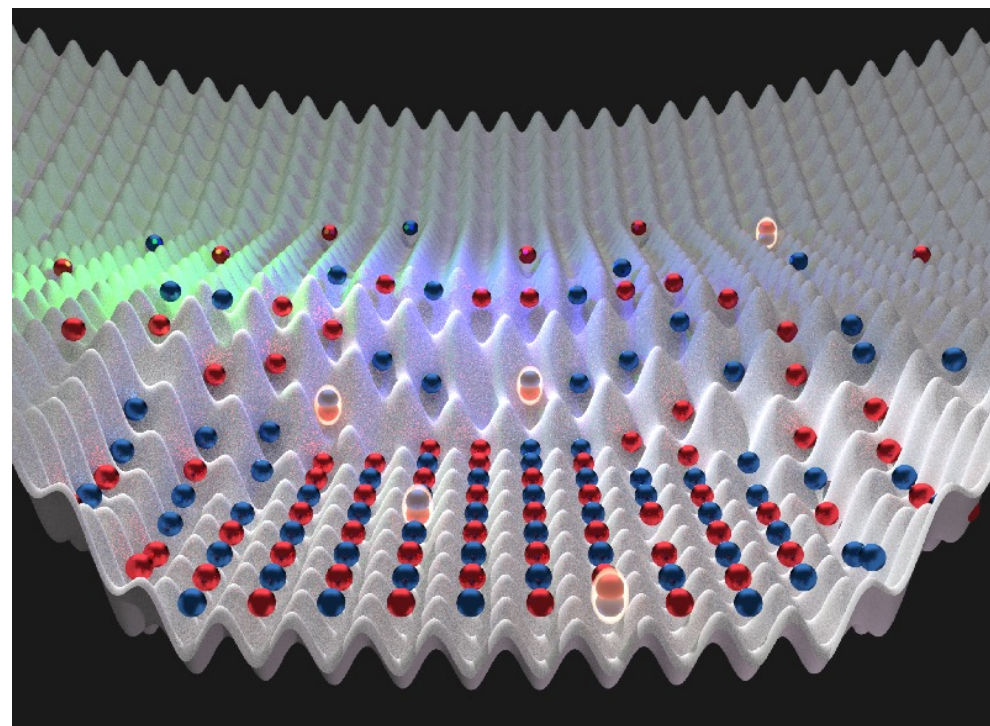
■ Two conditions for the quantum many-body systems

➡ (1) Interaction is short range

➡ (2) Energy per one particle is finite



Speed of the information propagation is finite



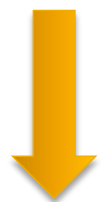
Cold atom experiment
(C. Chiu/Harvard University)

Two condition for the Lieb-Robinson bound

- Two conditions for the quantum many-body systems

➔ (1) Interaction is short range

➔ (2) Energy per one particle is finite



Speed of the information propagation is finite

[Long-range interactions]

Recent progress

Chen and Lucas, PRL 123, 250605 (2019).

Kuwahara and Saito, PRX 10, 031010 (2020)

Tran, et al., PRX, 11, 031016 (2021)

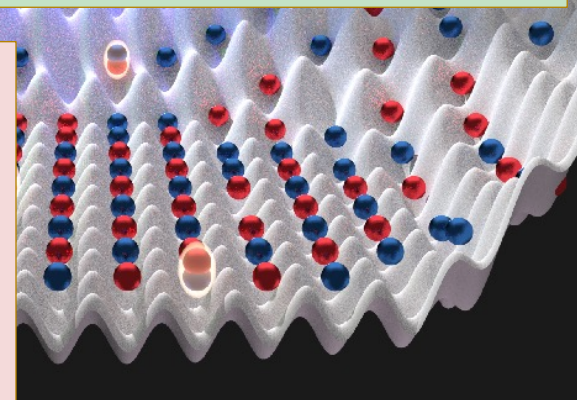
Kuwahara and Saito, PRL 126, 030604 (2021)

Tran, et al., PRL, 127, 160401 (2021)

[interacting Bosons]

Ubiquitous in cold atom experiment

→ Notoriously difficult !



Cold atom experiment

(C. Chiu/Harvard University)



Bosonic Lieb-Robinson bound

- Existence of examples with an infinite speed limit

J. Eisert and D. Gross, Phys. Rev. Lett. 102, 240501 (2009). QIP'09

➔ Need to consider natural cases. But, what is “natural” ?

- Mathematics for the bosonic Lieb–Robinson bound is scarce...

➔ N. Schuch, S. K. Harrison, T. J. Osborne, and J. Eisert, Phys. Rev. A **84**, 032309 (2011). QIP'11

Z. Wang and K. R. Hazzard, PRX Quantum **1**, 010303 (2020)

Our goal: establishing Lieb–Robinson bound for Bose–Hubbard model

➔ Partial success

T. Kuwahara, et al., PRL, **127**, 070403 (2021), Yin and Lucas, PRX, **12**, 021039 (2022), Faupin et al., PRL, **128**, 150602 (2022)

New Result

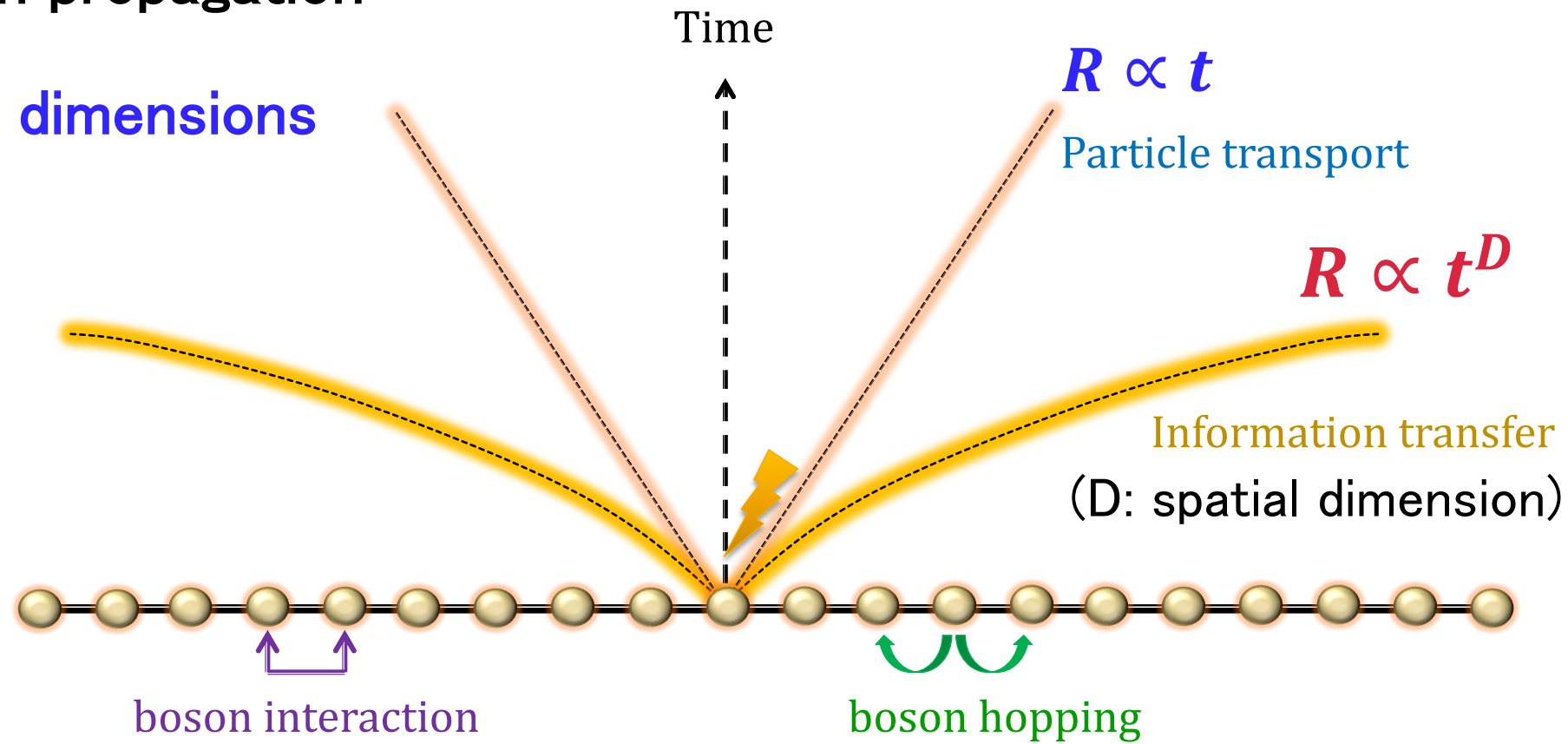
86

Kuwahara and Saito, arXiv:2206.14736

- Complete solution: optimal form of the effective light cone

- Speed of information propagation

→ Accelerating in high dimensions



New Result

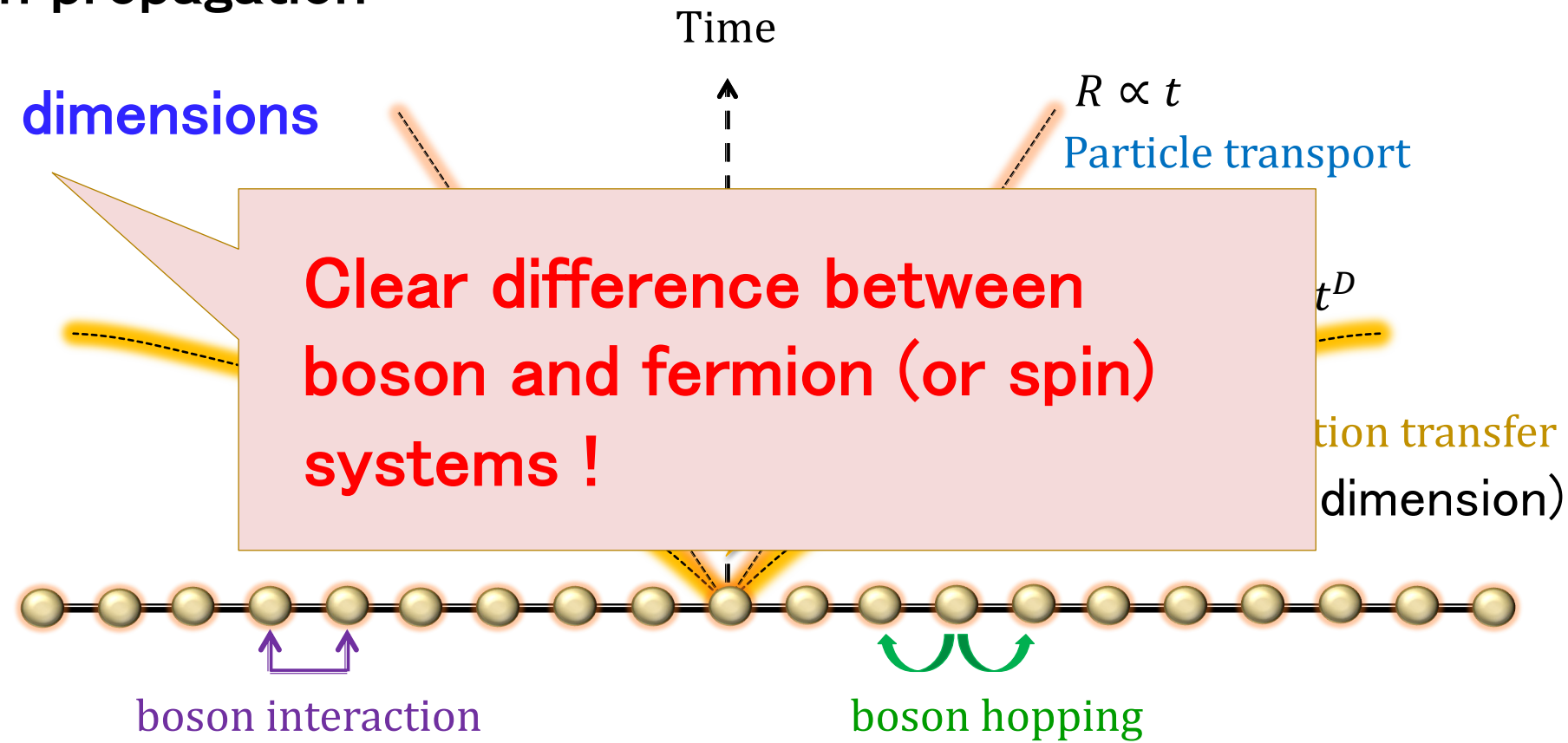
87

Kuwahara and Saito, arXiv:2206.14736

- Complete solution: optimal form of the effective light cone

- Speed of information propagation

→ Accelerating in high dimensions





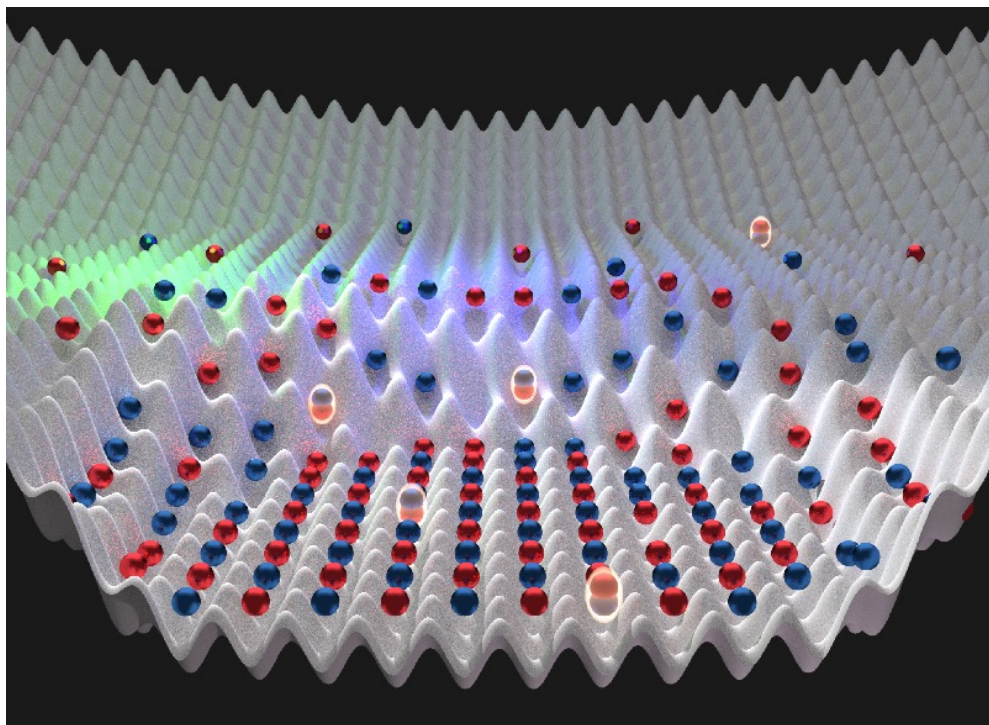
Application

88

- Gate complexity of quantum simulation

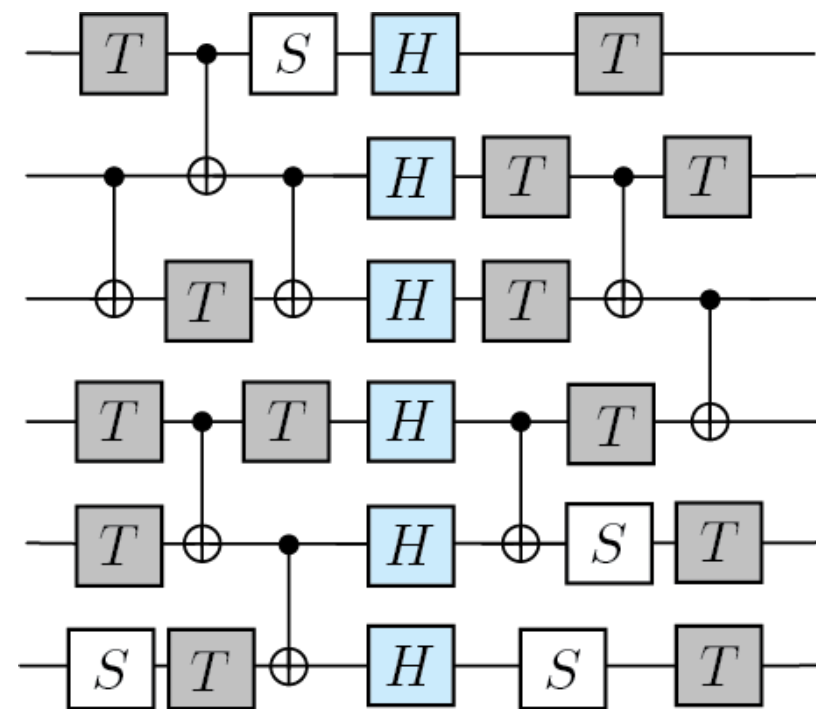
Kuwahara, Vu and Saito, arXiv:2206.14736

How many elementary quantum gates (e.g., CNOT, Hadamard, Phase shift gates) are sufficient to implement the quantum



?

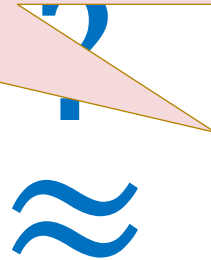
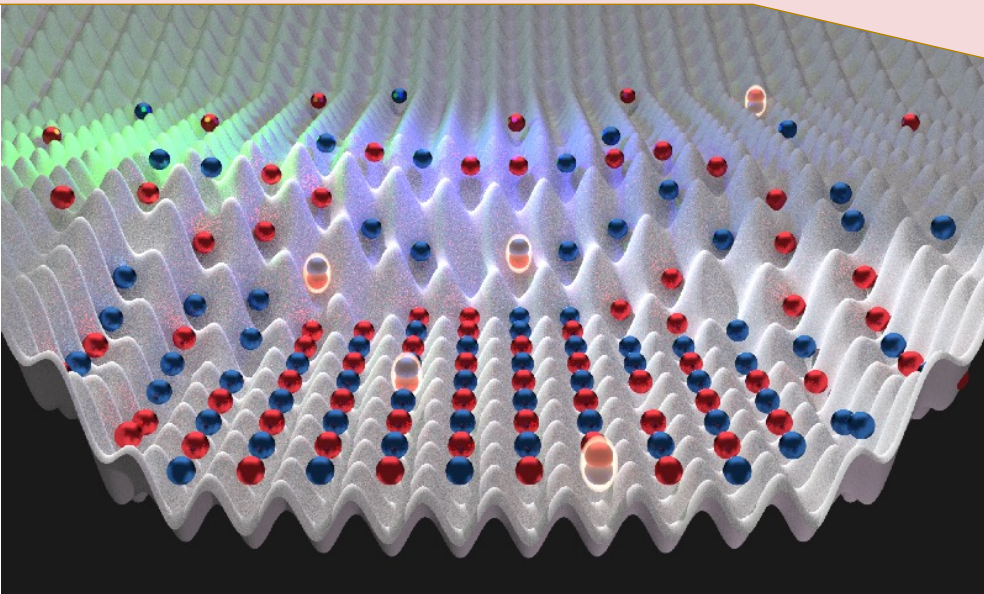
$\approx$



Quantum dynamics by the Bose–Hubbard model e^{-iHt} (N: system size, D: spatial dimension)

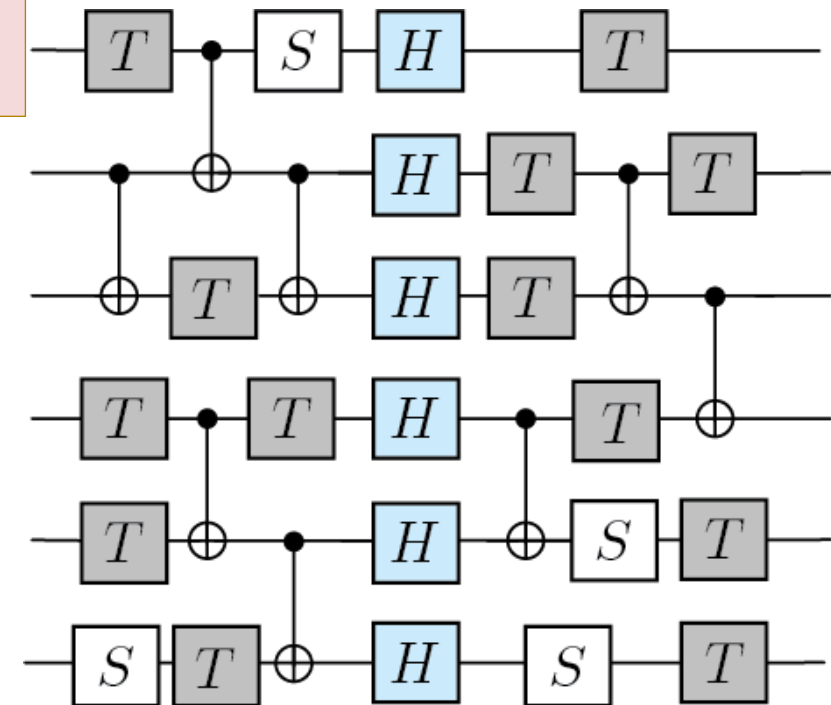
Sufficient number of quantum gates up to an error ε

$$Nt^{D+1} \text{polylog}(Nt/\varepsilon)$$



Kuwahara, Vu and Saito, arXiv:2206.14736

s (e.g., CNOT, Hadamard, complement the quantum



Future research

★ There are many other important problems !

- Quantum Markov conjecture → Quantum Gibbs sampling, SDP
- Area law conjecture → Density Matrix Renormalization Group method
- ✓ Bosonic Lieb–Robinson bound → Quantum simulator
- Finite–temperature topological order → Fault tolerant quantum computation
- Quantum PCP conjecture → Foundation of quantum computing

Future direction:

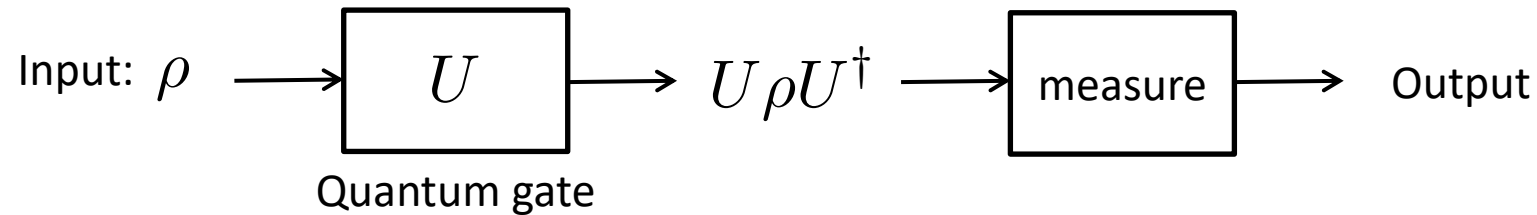
- Experimental observation of bosonic Lieb–Robinson bound (discussing with Fukuhara TL in RQC)



Supplemental slides (quantum circuit)

Quantum circuit and unitary operation

- Operations of Quantum computer: unitary map $\mathcal{H} \rightarrow \mathcal{H}$



- Quantum gates: composed of three basic quantum operations

Hadamard gate, $(\pi/8)$ -phase gate, Controlled NOT gate

- Computational time of the quantum computer

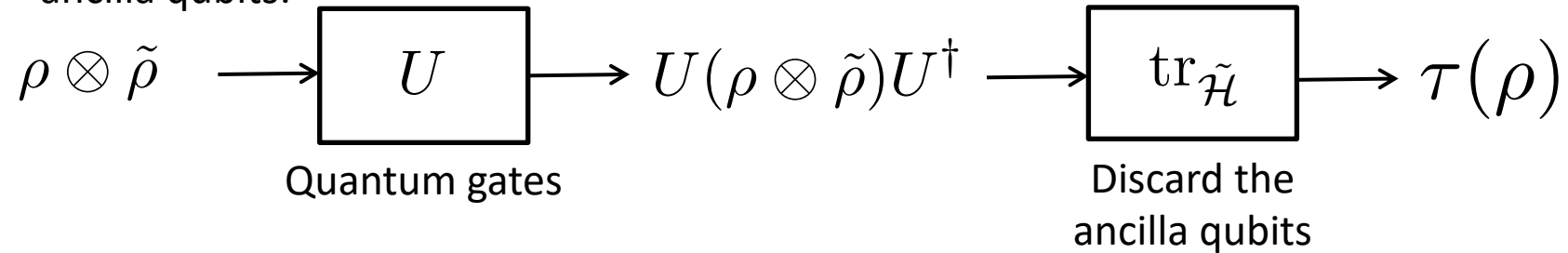
$\approx$ Necessary number of the basic quantum gates

CPTP map

(Completely Positive and Trace Preserving)

- The most general operations on the quantum computer

Input + ancilla qubits:



- τ : Completely Positive and Trace Preserving (CPTP) map

$$\tau(\rho) \succeq 0, \quad \text{tr}(\tau(\rho)) = \text{tr}(\rho)$$

- CPTP map

= Class of the operation which can be deterministically implemented by the quantum computer

Steinspring's dilation theorem (1955)

Supplemental slides

(Clustering of quantum correlation)

Decomposition of mixed state

95

- Any mixed state ρ

$$\rho = \sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j| = \sum_j p_j |\phi_j\rangle\langle\phi_j| \longrightarrow \rho = \sum_j \sqrt{p_j} |\psi_j\rangle\langle\psi_j| \sqrt{p_j} \quad \{|\psi_j\rangle\} : \text{arbitrary orthonormal bases}$$

- Quantum correlation and cluster

$$QC_\rho(O_A, O_B) := \inf_{\{p_i, \rho_i\}} \sum_i p_i |C_{\rho_i}(O_A, O_B)|$$

If we simply choose $|\psi_j\rangle$ as a product state,
 $\{|\phi_j\rangle = \sqrt{p_j} |\psi_j\rangle\} : \text{METTS ensemble}$

S. R. White, Phys. Rev. Lett. **102**, 190601 (2009)

- How to find the optimal base $\{|\psi_j\rangle\}$?

Choice of the decomposition

96

- Any mixed state ρ

$$\rho = \sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j| = \sum_j p_j |\phi_j\rangle\langle\phi_j| \longrightarrow \rho = \sum_j \sqrt{\rho} \underset{\parallel}{|\psi_j\rangle\langle\psi_j|} \sqrt{\rho} \quad \{|\psi_j\rangle\} : \text{arbitrary orthonormal bases}$$

- Expectation value $\langle\phi_j|O|\phi_j\rangle$

$$\langle\phi_j|O|\phi_j\rangle = \frac{1}{2p_j} \langle\psi_j|\{\rho, \mathcal{L}_O\}|\psi_j\rangle \quad \mathcal{L}_O := \sum_{s,s'} \frac{2\sqrt{\lambda_s\lambda_{s'}}}{\lambda_s + \lambda_{s'}} \langle\lambda_s|O|\lambda_{s'}\rangle |\lambda_s\rangle\langle\lambda_{s'}|$$

- If $[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] = 0$, we may choose $\{|\psi_j\rangle\}$ as simultaneous eigenstates for $\mathcal{L}_{O_A}, \mathcal{L}_{O_B}$

$$\longrightarrow \langle\phi_j|O_A|\phi_j\rangle\langle\phi_j|O_B|\phi_j\rangle = \alpha_{1,j}\alpha_{2,j}$$

$\alpha_{1,j}$: eigenvalue of $\mathcal{L}_{O_A}$
 $\alpha_{2,j}$: eigenvalue of $\mathcal{L}_{O_B}$

Choice of the decomposition

- Any mixed state ρ

$$\rho = \sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j| = \sum_j p_j |\phi_j\rangle\langle\phi_j| \longrightarrow \rho = \sum_j \sqrt{\rho} \underbrace{|\psi_j\rangle\langle\psi_j|}_{\parallel \sqrt{p_j} |\phi_j\rangle} \sqrt{\rho} \quad \{|\psi_j\rangle\} : \text{arbitrary orthonormal bases}$$

- Expectation value $\langle\phi_j|O|\phi_j\rangle$

$$\langle\phi_j|O|\phi_j\rangle = \frac{1}{2p_j} \langle\psi_j|\{\rho, \mathcal{L}_O\}|\psi_j\rangle$$

Can we have

$$\langle\phi_j|O_A O_B|\phi_j\rangle = \alpha_{1,j} \alpha_{2,j} ? \quad \text{NO!}$$

- If $[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] = 0$, we may choose $\{|\psi_j\rangle\}$ as simultaneous eigenstates for $\mathcal{L}_{O_A}, \mathcal{L}_{O_B}$



$$\langle\phi_j|O_A|\phi_j\rangle\langle\phi_j|O_B|\phi_j\rangle = \alpha_{1,j}\alpha_{2,j}$$

$\alpha_{1,j}$: eigenvalue of $\mathcal{L}_{O_A}$

$\alpha_{2,j}$: eigenvalue of $\mathcal{L}_{O_B}$

Choice of the decomposition

98

- Any mixed state ρ

$$\rho = \sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j| = \sum_j p_j |\phi_j\rangle\langle\phi_j| \longrightarrow \rho = \sum_j \sqrt{\rho} \underset{\parallel}{|\psi_j\rangle\langle\psi_j|} \sqrt{\rho} \quad \{|\psi_j\rangle\} : \text{arbitrary orthonormal bases}$$

- Expectation value $\langle\phi_j|O|\phi_j\rangle$

$$\langle\phi_j|O|\phi_j\rangle = \frac{1}{2p_j} \langle\psi_j|\{\rho, \mathcal{L}_O\}|\psi_j\rangle \quad \mathcal{L}_O := \sum_{s,s'} \frac{2\sqrt{\lambda_s\lambda_{s'}}}{\lambda_s + \lambda_{s'}} \langle\lambda_s|O|\lambda_{s'}\rangle |\lambda_s\rangle\langle\lambda_{s'}|$$

- If $[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] = 0$, we may choose $\{|\psi_j\rangle\}$ as simultaneous eigenstates for $\mathcal{L}_{O_A}, \mathcal{L}_{O_B}$

$$\longrightarrow \langle\phi_j|O_A O_B|\phi_j\rangle = \alpha_{1,j}\alpha_{2,j} + \frac{1}{4} \langle\phi_j|[\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}, \rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2}]|\phi_j\rangle$$

$\alpha_{1,j}$: eigenvalue of $\mathcal{L}_{O_A}$
 $\alpha_{2,j}$: eigenvalue of $\mathcal{L}_{O_B}$

Upper bound on quantum correlation 99

- Any mixed state ρ

$$\rho = \sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j| = \sum_j p_j |\phi_j\rangle\langle\phi_j|$$

Under the assumption of $[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] = 0$,
we upper-bound

$$\begin{aligned} QC_\rho(O_A, O_B) &= \inf_{\{p_i, \rho_i\}} \sum_i p_i |C_{\rho_i}(O_A, O_B)| \\ &\leq \frac{1}{4} \|[\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}, \rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2}]\| \end{aligned}$$

- Expectation value $\langle\phi_j|$

$$\langle\phi_j|O|\phi_j\rangle = \frac{1}{2p_j} \langle\psi_j|\{\rho, \mathcal{L}_O\}|\psi_j\rangle$$

$$\sum_{s,s'} \frac{\lambda_s \lambda_{s'}}{\lambda_s + \lambda_{s'}} \langle\lambda_s|O|\lambda_{s'}\rangle |\lambda_s\rangle\langle\lambda_{s'}|$$

$\alpha_{1,j}$: eigenvalue of $\mathcal{L}_{O_A}$
 $\alpha_{2,j}$: eigenvalue of $\mathcal{L}_{O_B}$

- If $[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] = 0$, we may choose $\{|\psi_j\rangle\}$ as simultaneous eigenstates for $\mathcal{L}_{O_A}, \mathcal{L}_{O_B}$

$$\longrightarrow \langle\phi_j|O_A O_B|\phi_j\rangle - \langle\phi_j|O_A|\phi_j\rangle\langle\phi_j|O_B|\phi_j\rangle = \frac{1}{4} \langle\phi_j|[\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}, \rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2}]|\phi_j\rangle$$

Upper bound on quantum correlation¹⁰⁰

- In general, **we don't have** $[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] = 0$ for non-commuting Hamiltonians

- Construct approximate $\tilde{\mathcal{L}}_{O_A}, \tilde{\mathcal{L}}_{O_B}$, s.t.

$$[\tilde{\mathcal{L}}_{O_A}, \tilde{\mathcal{L}}_{O_B}] = 0,$$

$$\|\mathcal{L}_{O_A} - \tilde{\mathcal{L}}_{O_A}\| \leq \delta_1, \quad \|\mathcal{L}_{O_B} - \tilde{\mathcal{L}}_{O_B}\| \leq \delta_2$$

$$\mathcal{L}_O := \sum_{s,s'} \frac{2\sqrt{\lambda_s \lambda_{s'}}}{\lambda_s + \lambda_{s'}} \langle \lambda_s | O | \lambda_{s'} \rangle |\lambda_s\rangle \langle \lambda_{s'}|$$
$$\rho = \sum_j \lambda_j |\lambda_j\rangle \langle \lambda_j|$$

- If we can find above operators, we can derive

$$QC_\rho(O_A, O_B) \leq 2\delta_1 + 2\delta_2 + \delta_1\delta_2 + \frac{1}{4} \|[\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}, \rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2}]\|$$

For $\rho = \rho_\beta$, the Lieb-Robinson bound plays key roles in the error estimation!

Application of Lieb-Robinson bound

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- Describing $\mathcal{L}_O$ using the time evolution with $\rho_\beta = \sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j|$

$$\mathcal{L}_O = \sum_{s,s'} \frac{2\sqrt{\lambda_s \lambda_{s'}}}{\lambda_s + \lambda_{s'}} \langle \lambda_s | O | \lambda_{s'} \rangle |\lambda_s\rangle\langle\lambda_{s'}| = \int_{-\infty}^{\infty} f_\beta(t) O(t) dt \quad f_\beta(t) := \frac{1}{\beta \cosh(\pi t / \beta)}$$

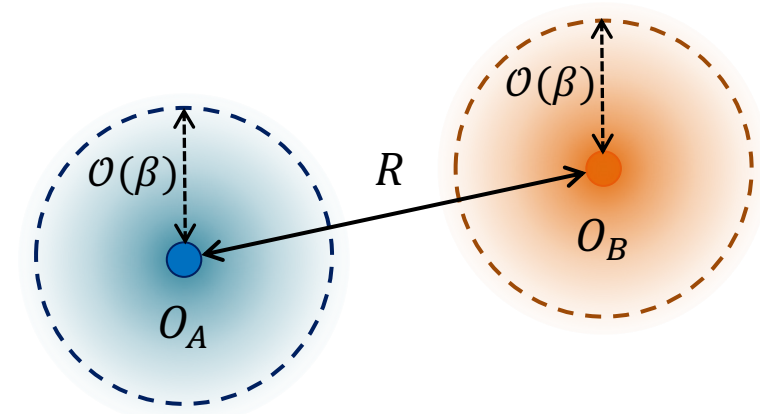
- Describing $\rho_\beta^{\pm 1/2} \mathcal{L}_O \rho_\beta^{\mp 1/2}$ using the time evolution

$$\rho_\beta^{\mp 1/2} \mathcal{L}_O \rho_\beta^{\pm 1/2} = \int_{-\infty}^{\infty} g_{\beta,\pm}(t) O(t) dt \quad g_{\beta,\pm}(t) = \delta(t) + \frac{-i}{\beta \sinh(\pi t / \beta)}$$

- $\mathcal{L}_{O_A}, \mathcal{L}_{O_B}, \rho_\beta^{\mp 1/2} \mathcal{L}_{O_A} \rho_\beta^{\pm 1/2}, \rho_\beta^{\mp 1/2} \mathcal{L}_{O_B} \rho_\beta^{\pm 1/2}$: quasi-local operator

→ $\mathcal{L}_{O_A}, \mathcal{L}_{O_B}$: approximately commute

$\rho_\beta^{\mp 1/2} \mathcal{L}_{O_A} \rho_\beta^{\pm 1/2}, \rho_\beta^{\mp 1/2} \mathcal{L}_{O_B} \rho_\beta^{\pm 1/2}$: approximately commute



Application of Lieb-Robinson bound

102

- Describing $\mathcal{L}_O$ using

$$\mathcal{L}_O = \sum_{s,s'} \frac{2\sqrt{\lambda_s \lambda_{s'}}}{\lambda_s + \lambda_{s'}} \langle \lambda_s | O | \lambda_{s'} \rangle$$

- Describing $\rho_\beta^{\pm 1/2}$

$$\rho_\beta^{\mp 1/2} \mathcal{L}_O \rho_\beta^{\pm 1/2} = \int_{-\infty}^{\infty} d\omega \tilde{\rho}_\beta(\omega) \mathcal{L}_O \tilde{\rho}_\beta(\omega)$$

By applying these approximate commutability to

$$QC_{\rho_\beta}(O_A, O_B) \leq 2\delta_1 + 2\delta_2 + \delta_1\delta_2 + \frac{1}{4} \|[\rho_\beta^{-1/2} \mathcal{L}_{O_A} \rho_\beta^{1/2}, \rho_\beta^{1/2} \mathcal{L}_{O_B} \rho_\beta^{-1/2}]\|$$

we derive the desired clustering theorem

$$QC_{\rho_\beta}(O_A, O_B) = \tilde{O}(|A| + |B|) e^{-R/\xi_\beta} \quad \xi_\beta = O(\beta)$$

- $\mathcal{L}_{O_A}, \mathcal{L}_{O_B}, \rho_\beta^{\mp 1/2} \mathcal{L}_{O_A} \rho_\beta^{\pm 1/2}, \rho_\beta^{\mp 1/2} \mathcal{L}_{O_B} \rho_\beta^{\pm 1/2}$: quasi-local operator

→ $\mathcal{L}_{O_A}, \mathcal{L}_{O_B}$: approximately commute

$\rho_\beta^{\mp 1/2} \mathcal{L}_{O_A} \rho_\beta^{\pm 1/2}, \rho_\beta^{\mp 1/2} \mathcal{L}_{O_B} \rho_\beta^{\pm 1/2}$: approximately commute

