

Improved thermal area law and quasi-linear time algorithm for quantum Gibbs states



Tomotaka Kuwahara
RIKEN AIP, RIKEN iTHEMS, Keio Univ.
QIP2021, 2nd Feb. (2021)



Joint work with
Alvaro Alhambra (Max Planck Institute) , Anurag Anshu (UC Berkley)

arXiv:2007.11174, to appear in Physical Review X

Outline

- Background
- Main results
- Proof techniques

Quantum Gibbs state

- Local Hamiltonian (system size : n , spatial dimension: d)

$$H = \sum_{\langle i,j \rangle} h_{i,j}, \quad \|h_{i,j}\| \leq 1$$

$\|\cdots\|$: operator norm

$\langle i,j \rangle$: pairs of adjacent spins

- Gibbs state : $\rho_\beta = e^{-\beta H} / \text{tr}(e^{-\beta H})$

- Target : **Efficient simulation of quantum Gibbs states**

→ Classical/Quantum simulation of thermal equilibrium

Verstraete, García-Ripoll and Cirac, PRL (2004). B-B Chen et al., PRX (2018).

M. Motta et al., Nature Physics (2020).

→ Quantum Machine learning

M. H. Amin et al., PRX (2018). Anshu, Arunachalam, Kuwahara and Soleimanifar, FOCS (2020).

→ Exponential speed up of Semidefinite Programming

Brandão and Svore, FOCS (2017). J. V. Apeldoorn et al., FOCS (2017)

High temperatures v.s. Low temperatures

■ Above a temperature threshold

- Clustering property (exponential decay of correlations)

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

- Approximate quantum Markov property

→ Efficient classical simulation (existence of FPTAS)

→ Construction by constant-depth quantum circuit

Kuwahara, Kato and Brandao, RRL (2020). M. Soreimanifar et al., STOC2020

■ Low-temperatures

- Computationally hard to simulate

F Barahona, J. Phys. A (1982). Aharonov, Arad, and Vidick ACM SIGACT (2013).

- Low temperature regime is important in practical applications

➡ $\beta = \mathcal{O}(\log(n))$ is required for Semidefinite Programming

Brandão and Svore, FOCS (2017).

High temperatures v.s. Low temperatures

■ Above a temperature threshold

- Clustering property (exponential decay of correlations)

. (2015).

- **What universally hold at low temperatures?**

S)
it

Kuwahara and Brandao, RRL (2020). M. Soreimanifar et al., STOC2020

■ Low-temperatures

- Computationally hard to simulate

F Barahona, J. Phys. A (1982). Aharonov, Arad, and Vidick ACM SIGACT (2013).

- Low temperature regime is important in practical applications

➡ $\beta = \mathcal{O}(\log(n))$ is required for Semidefinite Programming

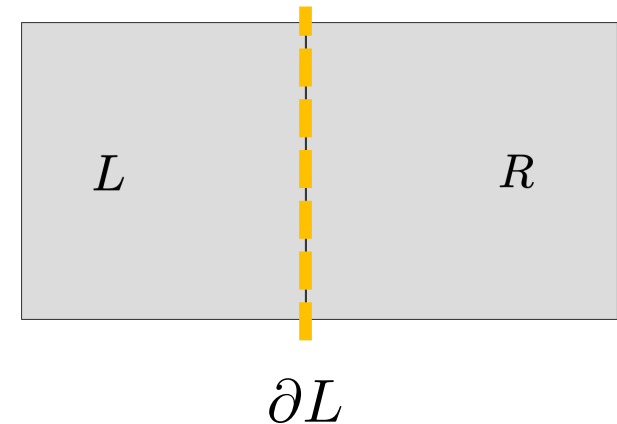
Brandão and Svore, FOCS (2017).

Thermal area law

- Mutual information

$$I(L : R)_{\rho_\beta} := S(\rho_\beta^L) + S(\rho_\beta^R) - S(\rho_\beta)$$

$\rho_\beta^L, \rho_\beta^R$: reduced density matrix

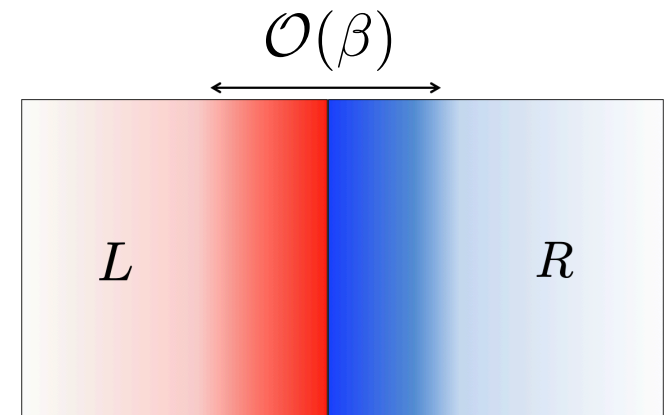


- Thermal Area law: $I(L : R)_{\rho_\beta} \lesssim \beta |\partial L|$

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

[Remarks]

- Derived from the minimization of the free energy by the quantum Gibbs state
- Quantum correlations spread over distance $\mathcal{O}(\beta)$
- Applicable to arbitrary dimensional systems



Physical interpretation in terms of imaginary time evolution

- Quantum Gibbs state

→ Imaginary time evolution for the uniform mixed state (i.e., $\rho_{\beta=0}$)

$$\rho_{\beta} \propto e^{-\beta H/2} \rho_{\beta=0} e^{-\beta H/2}$$

→ $I(L : R)_{\rho_{\beta}}$: entanglement generation by the imaginary-time evolution

→ $I(L : R)_{\rho_{\beta}} \lesssim \beta |\partial L|$

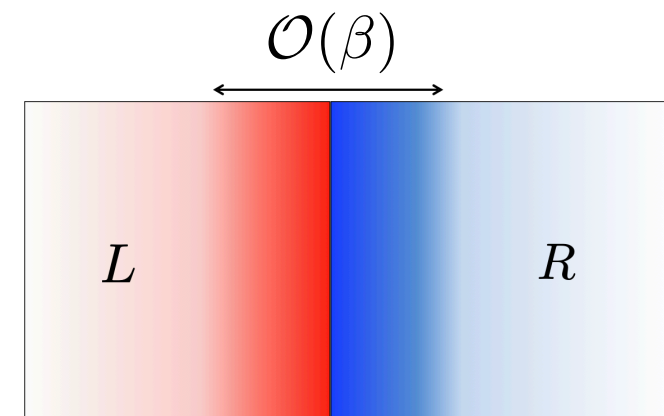
Entanglement rate is linear for the imaginary time



- Real time evolution: entanglement rate is linear (SIE theorem) K. V. Acoleyen et al., PRL (2013).

- Hastings' quantum belief propagation
→ quantum effect spreads over distance $\mathcal{O}(\beta)$

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



Physical interpretation in terms of imaginary time evolution

- Quantum Gibbs state

→ Imaginary time evolution

$$\rho_\beta \propto e^{-\beta H}$$

→ $I(L : R)_{\rho_\beta}$:

→ $I(L : R)_{\rho_\beta} \lesssim \beta |\partial L|$

Entanglement rate is linear for the imaginary time

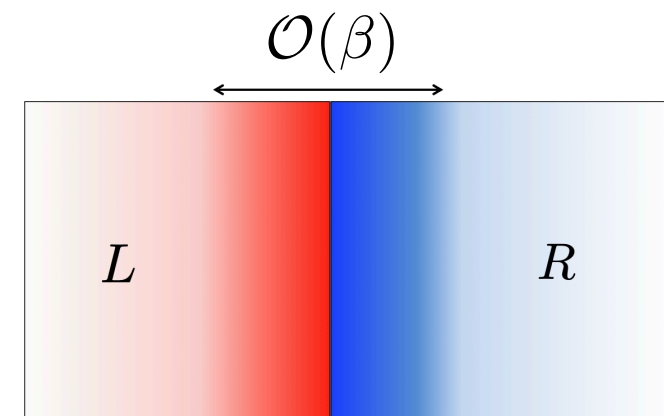


- Real time evolution: entanglement rate is linear (SIE theorem) K. V. Acoleyen et al., PRL (2013).

- Hastings' quantum belief propagation
→ quantum effect spreads over distance $\mathcal{O}(\beta)$

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

Our result: Entanglement rate is sublinear unlike the real time evolution!



Outline

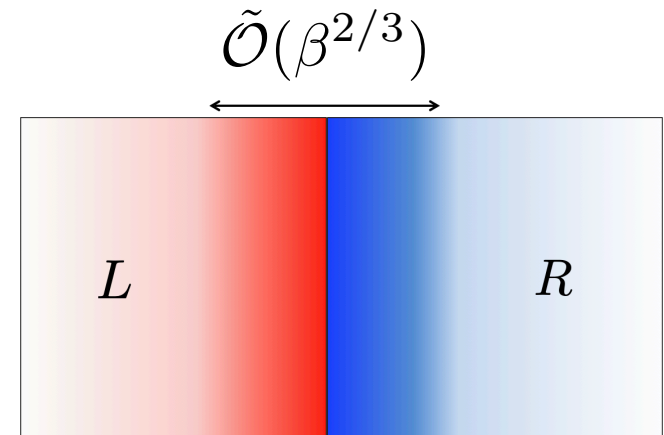
- Background
- Main results
- Proof techniques

Our result

■ Improved thermal area law

$$I(L : R)_{\rho_\beta} = \tilde{\mathcal{O}}(\beta^{2/3} |\partial L|)$$

$$\tilde{\mathcal{O}}(x) = \mathcal{O}(x \log x)$$



→ Applicable to all the finite-dimensional systems

→ Quantum correlations spread over distance $\tilde{\mathcal{O}}(\beta^{2/3})$

→ It is not clear whether the exponent (2/3) can be further improved.

What is the optimal γ such that $I(L : R)_{\rho_\beta} \lesssim \beta^\gamma |\partial L|$?

→ Gottesman-Hastings example : 1D Gibbs state such that $\gamma \geq 1/5$

$$1/5 \leq \gamma \leq 2/3$$

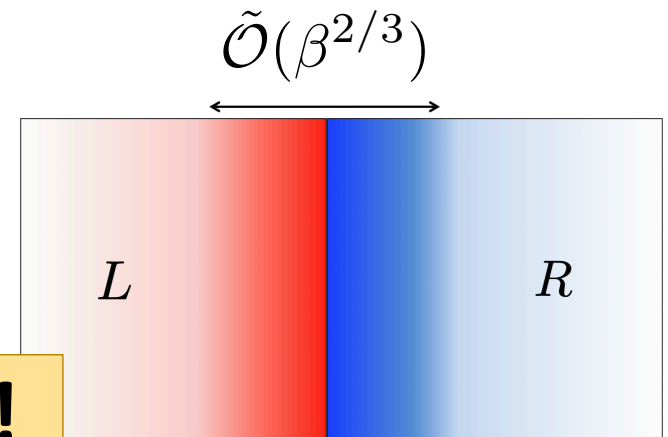
Gottesman and Hastings, NJP (2010).

Our result

- Improved thermal area law

$$I(L : R)_{\rho_\beta} = \tilde{\mathcal{O}}(\beta^{2/3} |\partial L|)$$

$$\tilde{\mathcal{O}}(x) = \mathcal{O}(x \log x)$$



We can get practical implications!

MPO approximation

and

Quasi-linear time algorithm

...ner improved.

What is the optimal γ such that $I(L : R)_{\rho_\beta} \lesssim \beta^\gamma |\partial L|$?

➔ Gottesman-Hastings example : 1D Gibbs state such that $\gamma \geq 1/5$

$$1/5 \leq \gamma \leq 2/3$$

Gottesman and Hastings, NJP (2010).

Our result: MPO approximation by sublinear bond dimension

- Matrix product operator approximation (D : bond dimension)

$$M_D = \sum_{\substack{s_1, s_2, \dots, s_n=1 \\ s'_1, s'_2, \dots, s'_n=1}}^{\varsigma} \text{tr} \left(A_1^{[s_1, s'_1]} A_2^{[s_2, s'_2]} \dots A_n^{[s_n, s'_n]} \right) |s_1, s_2, \dots, s_n\rangle \langle s'_1, s'_2, \dots, s'_n|,$$

ς : dimension of local Hilbert space

$A_j^{[s_j, s'_j]}$: $D \times D$ matrix

- MPO approximation for 1D quantum Gibbs state**

$$\|\rho_\beta - M_D\|_1 \leq \epsilon \quad \text{if} \quad D = e^{\tilde{O}(\beta^{2/3}) + \tilde{O}(\sqrt{\beta \log(n/\epsilon)})}$$

➡ For $\beta = o(\log(n))$, **sublinear bond dimension** is enough for good approximation

➡ Better than the state-of-the-art estimation as $D = (n/\epsilon)^{\mathcal{O}(\beta)}$

M.B. Hastings, PRB **73**, 085115 (2006).

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

A. Molnar et al., PRB (2015).

Our result: quasi-linear time algorithm

- Existence of MPO approximation and finding it are different problem

➡ (Imaginary TEBD algorithm) truncating the bond dimension iteratively

Verstraete, García-Ripoll and Cirac, PRL (2004).

B-B Chen et al., PRX (2018).

No efficiency guarantees!!!

- Cluster-expansion-based algorithm: Computational cost= $n^{\mathcal{O}(\beta)}$
for finding the MPO s.t. $\|\rho_\beta - M_D\|_1 \leq 1/\text{poly}(n)$

A. Molnar et al., PRB (2015).

➡ Polynomial time complexity as long as $\beta = \mathcal{O}(1)$

- **Our new algorithm: Computational cost= $n \exp \left[\tilde{\mathcal{O}} \left(\sqrt{\beta \log(n)} \right) \right]$
for finding the MPO s.t. $\|\rho_\beta - M_D\|_1 \leq 1/\text{poly}(n)$**

➡ Quasi-linear time complexity as long as $\beta = o(\log(n))$

Outline

- Background
- Main results
- Proof techniques

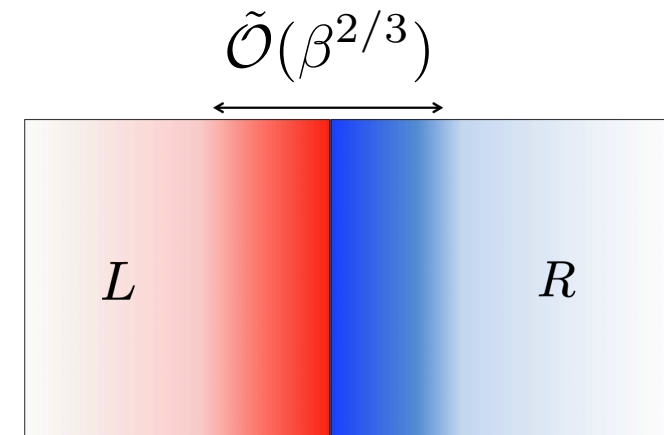
Imaginary-time evolution v.s. random walk

- Improved thermal area law: sub-ballistic propagation of entanglement by imaginary time evolution

➡ Rigorously justified?

- Toy model: tight-binding model

$$H = \sum_{x=-R}^R (|x\rangle\langle x+1| + |x+1\rangle\langle x| - 2|x\rangle\langle x|)$$



➡ Real-time evolution: ballistic propagation of the particle

➡ Imaginary-time evolution: diffusive propagation of the particle

Schrodinger eq. is formally equivalent to the random walk eq.

Imaginary-time evolution v.s. random walk

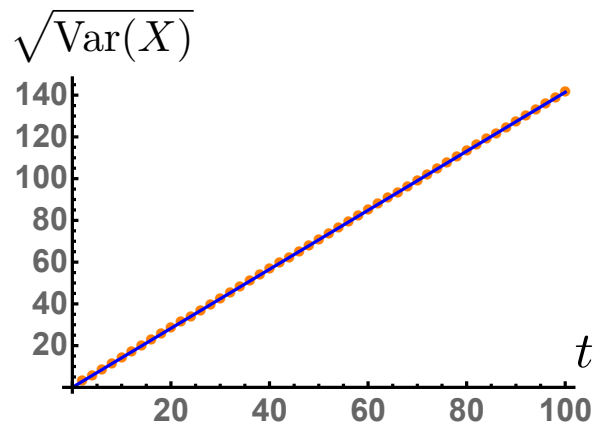
- Improved thermal area law:
sub-ballistic propagation of entanglement by imaginary time evolution

➡ Rigorously justified?

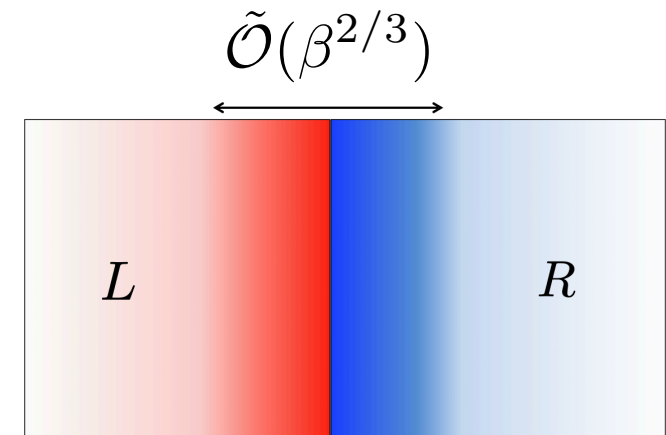
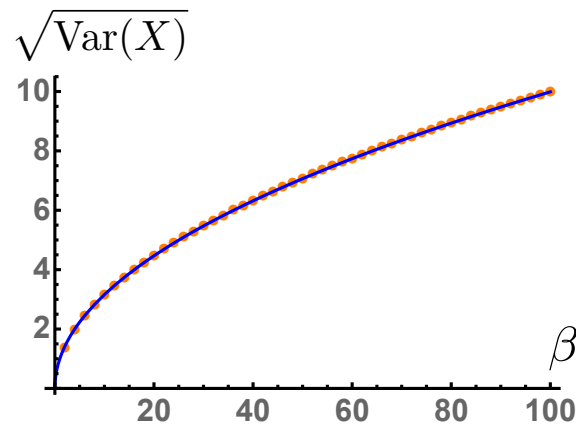
- Toy model: tight-binding model

$$H = \sum_{x=-R}^R (|x\rangle\langle x+1| + |x+1\rangle\langle x| - 2|x\rangle\langle x|)$$

(real time)



(Imaginary time)



Imaginary-time evolution v.s. random walk

- Improved thermalization
- sub-ballistic propagation

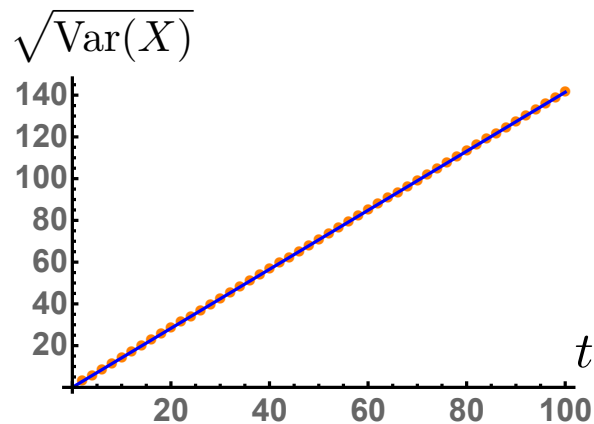
How to generalize to many-body Hamiltonian?

→ Rigorously justified

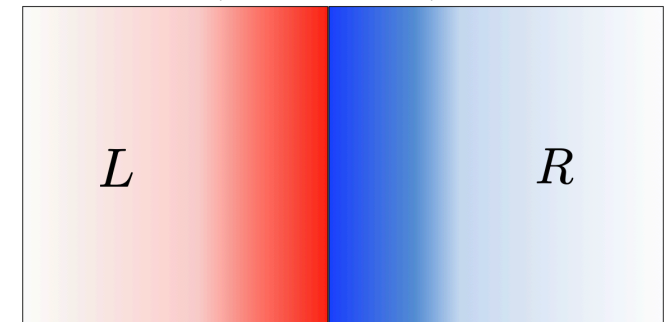
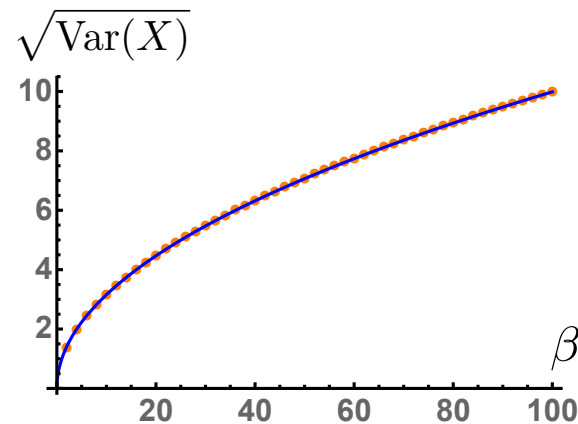
- Toy model: tight-binding model

$$H = \sum_{x=-R}^R (|x\rangle\langle x+1| + |x+1\rangle\langle x| - 2|x\rangle\langle x|)$$

(real time)



(Imaginary time)



Imaginary-time evolution v.s. random walk

- Polynomial expansion by Sachdeva and Vishnori

Sushant Sachdeva and Nisheeth K. Vishnoi, “*Faster Algorithms via Approximation Theory*,” Foundations and Trends® in Theoretical Computer Science **9**, 125– 210 (2014).

→ Expanding e^{-x} ($x \in [0, b]$, $b \in \mathbb{N}$) by Chebyshev polynomials

$$\rightarrow e^{-\frac{b}{2}(1+y)} = \sum_{r_b=-\infty}^{\infty} P(r_b) T_{r_b}(y) \quad x = \frac{b(1+y)}{2} \quad (y \in [-1, 1])$$

→ $P(r_b)$ is **constructed from the b-step random walk**

$$P(r_b) \approx 0 \quad \text{for} \quad r_b \gg \sqrt{b}$$

→ e^{-x} is well approximated by
 $\mathcal{O}(\sqrt{b})$ -degree polynomial !

Imaginary-time evolution v.s. random walk

■ Polynomial expansion by Sachdeva and Vishnori

Sus
and

Quantum Gibbs state: $x = \beta H$, $b = \|\beta H\| = \mathcal{O}(\beta n)$

▪ \sqrt{b} is still too large..., also the approximation holds only in terms of operator norm

▪ For the proof, combining several techniques of

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

Connection of approximations by general Schatten norms

Refined Schmidt rank estimation, etc.,

A. Molnar et al., PRB (2015).

Arad et al., arXiv:1301.1162, Anshu et al., STOC (2020),

→ e^{-x} is well approximated by
 $\mathcal{O}(\sqrt{b})$ -degree polynomial !

Quasi-linear time algorithm: Block decomposition of Gibbs state

- Haah-Hastings-Kohtari-Low (FOCS2018, QIP2019)

➡ Decomposition of the unitary time operator based on the Lieb-Robinson bound

- Similar idea for the quantum Gibbs state

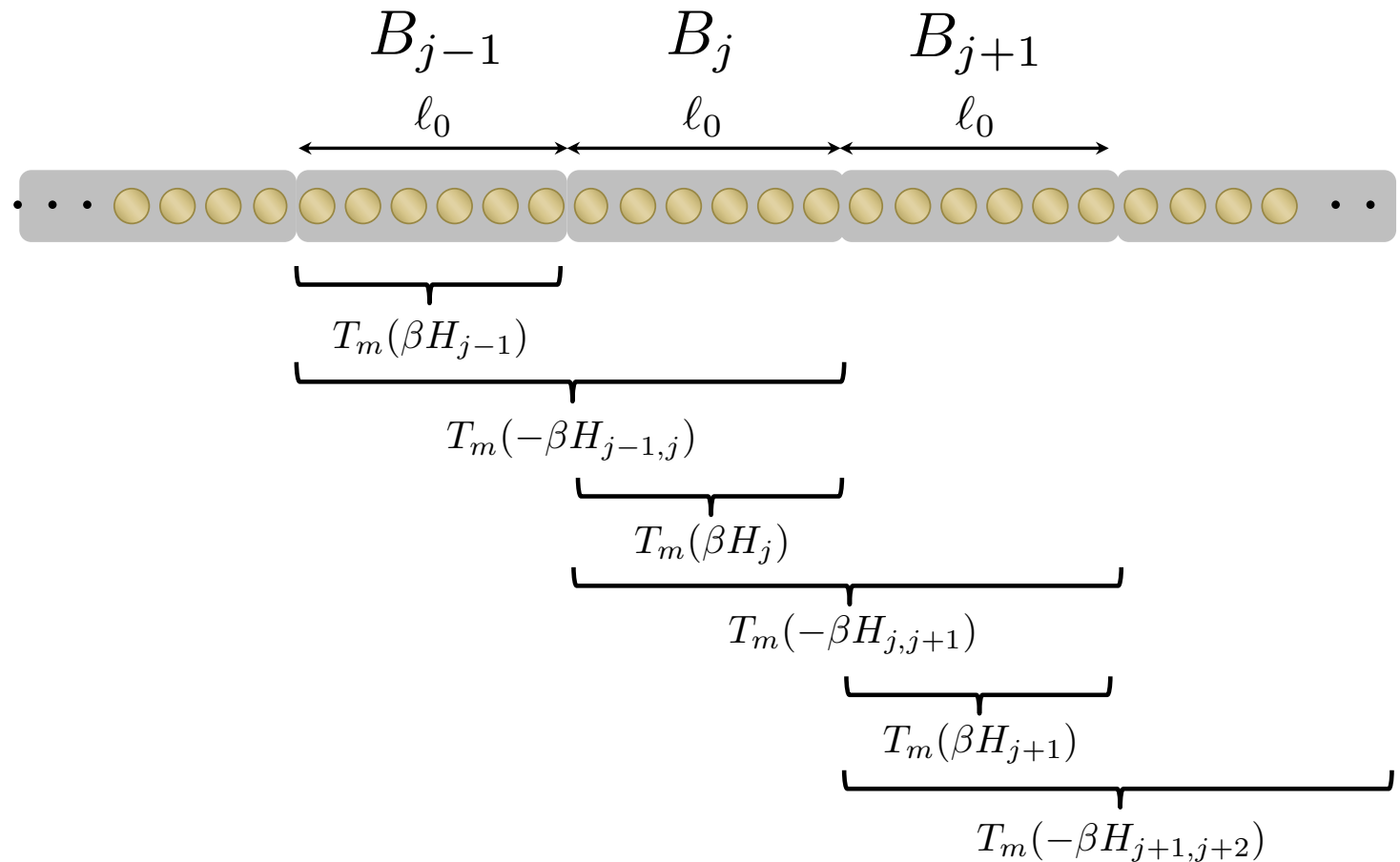
➡ Decomposing the Gibbs state as $e^{-\beta H} = (e^{-\beta_0 H})^{\beta/\beta_0}$

β_0 : sufficiently small such that the imaginary-time Lieb-Robinson bound exists

➡ Approximate $e^{-\beta_0 H}$ by **product of appropriate polynomials**

$$e^{-\beta_0 H} \approx M_{\beta_0} = T_m(-\beta_0 H_1) T_m(\beta_0 H_1) T_m(-\beta_0 H_{1,2}) T_m(\beta_0 H_2) T_m(-\beta_0 H_{2,3}) T_m(\beta_0 H_3) \cdots$$

Quasi-linear time algorithm: Block decomposition of Gibbs state



$$e^{-\beta_0 H} \approx M_{\beta_0} = T_m(-\beta_0 H_1) T_m(\beta_0 H_1) T_m(-\beta_0 H_{1,2}) T_m(\beta_0 H_2) T_m(-\beta_0 H_{2,3}) T_m(\beta_0 H_3) \cdots$$

Quasi-linear time algorithm: Block decomposition of Gibbs state

- Haah-Hastings-Kohtari-Low (FOCS2018, QIP2019)

➡ Decomposition of the unitary time operator based on the Lieb-Robinson bound

- Similar idea for the quantum Gibbs state

➡ Decomposing the Gibbs state as $e^{-\beta H} = (e^{-\beta_0 H})^{\beta/\beta_0}$

β_0 : sufficiently small such that the imaginary-time Lieb-Robinson bound exists

➡ Approximate $e^{-\beta_0 H}$ by **product of appropriate polynomials**

$$e^{-\beta_0 H} \approx M_{\beta_0} = T_m(-\beta_0 H_1) T_m(\beta_0 H_1) T_m(-\beta_0 H_{1,2}) T_m(\beta_0 H_2) T_m(-\beta_0 H_{2,3}) T_m(\beta_0 H_3) \cdots$$

- Approximation error is estimated by the imaginary-time Lieb-Robinson bound

- Bond dimension is derived by using the technique by Arad-Kitaev-Landau-Vazirani

Arad et al., arXiv:1301.1162

➡ Desired time complexity

Summary

- Original thermal area law is improved as

$$I(L : R)_{\rho_\beta} \lesssim \beta |\partial L| \rightarrow I(L : R)_{\rho_\beta} \lesssim \beta^{2/3} |\partial L|$$

Sub-ballistic entanglement propagation by imaginary time evolution

- Bond dimension for approximation by the MPO is improved as

$$D = (n/\epsilon)^{\mathcal{O}(\beta)} \rightarrow D = e^{\tilde{\mathcal{O}}(\beta^{2/3}) + \tilde{\mathcal{O}}(\sqrt{\beta \log(n/\epsilon)})}$$

Sub-linear bond dimension is enough for the approximation

- Time complexity for simulating the 1D Gibbs state is improved as

$$n^{\mathcal{O}(\beta)} \rightarrow n \exp \left[\tilde{\mathcal{O}} \left(\sqrt{\beta \log(n)} \right) \right]$$

Quasi-linear time algorithm is achieved

Thank you for listening