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

T. Kuwahara, Á. M. Alhambra, A. Anshu

I. MOTIVATION AND BACKGROUND

In the past few decades, one of the triumphs in the domain of quantum information theory has been the characterization of quantum many-body systems using information-theoretic methods. The advancements have enabled rigorous analysis of various heuristic classical and quantum algorithms, such as the Density Matrix Renormalization Group algorithm [1, 2]. Much of this success has come from the information-theoretic characterization of the correlations present between quantum systems. Motivated by this idea, the fundamental question answered in this study is the following: *How much information is shared between two complementary parts of a system?* This simple problem has received significant interest from researchers from various backgrounds, since it is closely related to the quest for efficient algorithms to simulate physical systems. Answers have, in many instances, established profound connections between information theory, computer science, and physics.

The amount of the information in quantum states is measured in terms of various quantities (e.g., entanglement entropy, mutual information, entanglement of purification, etc.). One of the most famous examples is the area law of the entanglement entropy in non-critical ground states [3, 4]. It argues that when we decompose a total system into two subsystems, the shared information is proportional to the boundary area of the subregion. Despite the extensive studies that have been conducted over the past twenty years, a rigorous proof remains completely open beyond 1D quantum systems. On the other hand, the area law in thermal equilibrium (hereafter referred to as the thermal area law) has been already established in a much simpler manner, in 2008 [5]. This work shows that the mutual information between two subsystems L and R is upper-bounded by the boundary area $|\partial L|$ times the inverse temperature β, namely $\beta|\partial L|$. This suggests that the non-local quantum effect increases linearly with the inverse temperature β. The result was expected to be tight as it seems to be physically natural and consistent with the theory of belief propagation [6] which argues the quantum non-locality spreads over a distance of $\mathcal{O}(\beta)$ at finite temperatures. Subsequent studies [7–9] have also shown that the time complexity of preparing a classical description of 1D thermal states on n spins is bounded by $n^{\mathcal{O}(\beta)}$. The linear dependence of the exponent on β is thus consistent with that of the area law $\beta|\partial L|$. This highlights the very close connection between area laws and algorithms for many-body systems.

II. SUMMARY OF MAIN RESULTS AND APPLICATIONS

Improved thermal area law.— In this work, we establish a new area law for mutual information in arbitrary quantum Gibbs states, which defies the intuition stemming out of most previous works. Our new area law improves the temperature dependence from $\mathcal{O}(\beta)$ to $\mathcal{O}(\beta^{2/3})$.

Theorem 1. For an arbitrary cut $\Lambda = L \cup R$, the mutual information $I_\beta(L:R)$ is upper-bounded by

$$I(L:R)_{\rho_\beta} \leq C\beta^{2/3}|\partial\Lambda| \left(\log^{2/3}(|\partial\Lambda|) + \log(\beta)\right), \tag{1}$$

where C is a constant of $\mathcal{O}(1)$. In particular, for one-dimensional systems ($|\partial\Lambda| = 1$), we have

$$I(L:R)_{\rho_\beta} \leq C\beta^{2/3}\log(\beta) = \tilde{\mathcal{O}}(\beta^{2/3}). \tag{2}$$

The central technical aspects of our study are a refined polynomial approximation of the exponential function and a Schmidt rank analysis of the polynomials of Hamiltonian. These enable powerful ideas from approximation theory to be used for studying quantum Gibbs states. Our techniques also allow us to put bounds on other measures of correlations, namely:

- The so-called Renyi entanglement of purification [10, 11], which we show is bounded by

$$E_{p,\alpha}(\rho) \leq \tilde{C}_0 \max\left[\beta^{2/3}\log(\beta), \frac{(1-\alpha)\beta}{\alpha}\log\left(\frac{\beta}{\alpha}\right)\right], \tag{3}$$

  where $\tilde{C}_0$ is an $\mathcal{O}(1)$ constant.

- Convex combination of matrix product states [12] (which has been linked to the success of certain algorithms for non-equilibrium dynamics [13]). That is, there exists a set of MPS $\{|M_i\rangle\}_{i=1}^{\mathcal{D}_\Lambda}$ ($\mathcal{D}_\Lambda$: total Hilbert space dimension) with bond dimension D such that

$$\left\|\rho_\beta - \sum_{i=1}^{\mathcal{D}_\Lambda} p_i |M_i\rangle\langle M_i|\right\|_1 \leq \epsilon, \qquad \text{and} \qquad D = \exp\left[\mathcal{O}\left(\max\left[\beta^{2/3}, \sqrt{\beta\log(\beta n/\epsilon)}\right]\right)\right]. \tag{4}$$

At the conceptual level, our result identifies a fundamental difference between imaginary time evolution and real time evolution. Based on the well-known small-incremental-entangling theorem [14–17], the entropy production via real time evolution is proportional to time. On the other hand, our result implies that *the entropy production via imaginary time evolution is sublinear in imaginary time*, thus spreading in a sub-ballistic fashion. In experimental level, imaginary time evolution has been realized using the Noisy Intermediate Scale Quantum (NISQ) device [20, 21]. Our result suggests the possibility of the behavior of the imaginary time evolution being more "spooky" than ever considered, which is of interest both in theoretical and experimental studies. We partially explain this point by focusing on the fact that imaginary time evolution has a strong relationship with random walks. In fact, this random walk aspect is a key ingredient in the polynomial approximations used here (see Sec. III).

To summarize our contribution, we shed light on the new fundamental problem of "*what is the critical γ_c for establishing the thermal area law scaling of β^{γ_c} in generic quantum many-body systems.*" We expect future studies to further pursue the value of γ_c (which we conjecture to be 1/2) and also, consequently, obtain better approximation algorithms. Importantly, the improvement cannot be below 1/5, which we show by providing an explicit family of examples [22]. Our work shows that the established thermal area law, which had been believed to be tight, can in fact be improved. This shows that previous intuitions on this subject may have been incomplete, and that there is a deeper structure that warrants exploration. We expect this pursuit will contribute to our better understanding of the structure an simulation of quantum thermal states, which are of the greatest importance to both quantum condensed matter and quantum simulation and computation.

Quasi-linear time algorithm for 1D quantum Gibbs state.— The improved area law is not only a topic of fundamental interest but also offers various practical applications for qualitatively improving important established results. Most importantly, in the computation of 1D quantum Gibbs states at arbitrary temperatures, our result achieves the first improvement *from polynomial time complexity to quasi-linear time complexity*, consistent with what is expected from heuristic algorithms. Thus far, there was no rigorous proof for a quasi-linear scaling of such an algorithm. The approach is based on approximations of thermal states with MPOs. The result is as follows.

Theorem 2. For arbitrary β, we can efficiently compute a matrix product operator M_β which approximates $e^{-\beta H}$ in the sense that $\|M_\beta - e^{-\beta H}\|_1 \leq \epsilon\|e^{-\beta H}\|_1$ ($\epsilon \leq 1$) where the bond dimension of M_β is given by $\exp(Q_\epsilon)$ with $Q_\epsilon := C\max\left[\beta, \sqrt{\beta\log(n/\epsilon)}\right]\log[\beta\log(n/\epsilon)]$ (C: constant). Also, the computational time to calculate M_β is $n\beta\exp(Q_\epsilon)$. When $\beta \lesssim \log(n/\epsilon)$ and $\epsilon = 1/\mathrm{poly}(n)$, the time complexity is quasi-linear with respect to the system size n:

$$n\exp\left[\tilde{\mathcal{O}}\left(\sqrt{\beta\log(n)}\right)\right]. \tag{5}$$

With our technique, we can also obtain the quasi-linear time complexity $ne^{\tilde{\mathcal{O}}(|t|)+\tilde{\mathcal{O}}(\sqrt{|t|\log n})}$ for the simulation of real time evolution e^{iHt}, which is better than the existing result [18] for $t = o(\log(n))$.

This is the first rigorous algorithmic result in many-body physics that achieves a runtime close to that of practical (but heuristic) methods, such as TEBD or METTS. This algorithm, which can be considered as the imaginary-time version of [23], converges in quasi-linear time, a scaling that matches the performance of some of the leading numerical techniques.

III. KEY TECHNIQUES

Improved thermal area law implies that the entanglement generation rate is sublinear with the imaginary time. So, it also indicates that the imaginary time evolution inherently induces a sub-ballistic propagation of entanglement. In order to rigorously justify it, we utilize the polynomial expansion by Sachdeva and Vishnori [19]. The point of their analysis is expanding of the exponential function e^{-x} ($x \in [0, b]$) by using the Chebyshev polynomials: $e^{-x} = \sum_{r_b=-\infty}^{\infty} P(r_b) T_{r_b}(y)$, where $x = b(1+y)/2$ ($y \in [-1, 1]$) and T_r is the rth order Chebyshev polynomial. Here, the coefficient $P(r_b)$ is constructed from the b-step random walk and is strongly concentrated around $r_b \approx \sqrt{b}$ (see Eq. (17) in the technical paper). In applying it to the quantum Gibbs state, we choose x as βH and b is equal to the norm of βH, which is as large as βn. However, the polynomial degree $\sqrt{b} \approx \sqrt{\beta n}$ is still too large. For the proof of the improved thermal area law, we need a combinatorial approach from several techniques (Lemmas 13, 14, 15 and 16 in the technical paper) such as the quantum belief propagation [6], connection of approximations by general Schatten-p norms [8], refined Schmidt rank estimations [24, 25] and so on.

Finally, we will show the essential idea to obtain the quasi-linear time algorithm (Theorem 2). Our method is similar to the Haah-Hastings-Kohtari-Low algorithm [23]. The key technique therein is the block decomposition of the unitary time operator based on the Lieb-Robinson bound [26]. We adopt a similar idea for the quantum Gibbs state. We first decompose the Gibbs state to the pieces of high-temperature Gibbs state $e^{-\beta_0 H}$, namely $e^{-\beta H} = (e^{-\beta_0 H})^{\beta/\beta_0}$. Here, the inverse temperature β_0 is sufficiently small such that the imaginary-time Lieb-Robinson bound exists. Furthermore, we approximate the quantum Gibbs state of $e^{-\beta_0 H}$ by using a product of appropriate polynomials (Fig. 1):

$$e^{-\beta_0 H} \approx M_{\beta_0} = \prod_{j=1}^{n} T_m(\beta_0 H_{j-1}) T_m(-\beta_0 (H_{j-1} + H_j)),$$

where the system is decomposed into blocks of length $l_0 = \mathcal{O}(\log(n/\epsilon))$, H_j is the Hamiltonian in the jth block, and $T_m(x) = \sum_{s=0}^{m} x^m/m!$ is the truncated Taylor expansion of order $m = \mathcal{O}(\log(n/\epsilon))$. Now, the approximation error is estimated by using the imaginary-time Lieb-Robinson bound, and the bond dimension of M_{β_0} is derived by using the technique in Ref. [24] (see Proposition 4 and Lemma 5 in the technical paper, respectively). By combining these analyses, we can achieve the desired time complexity.

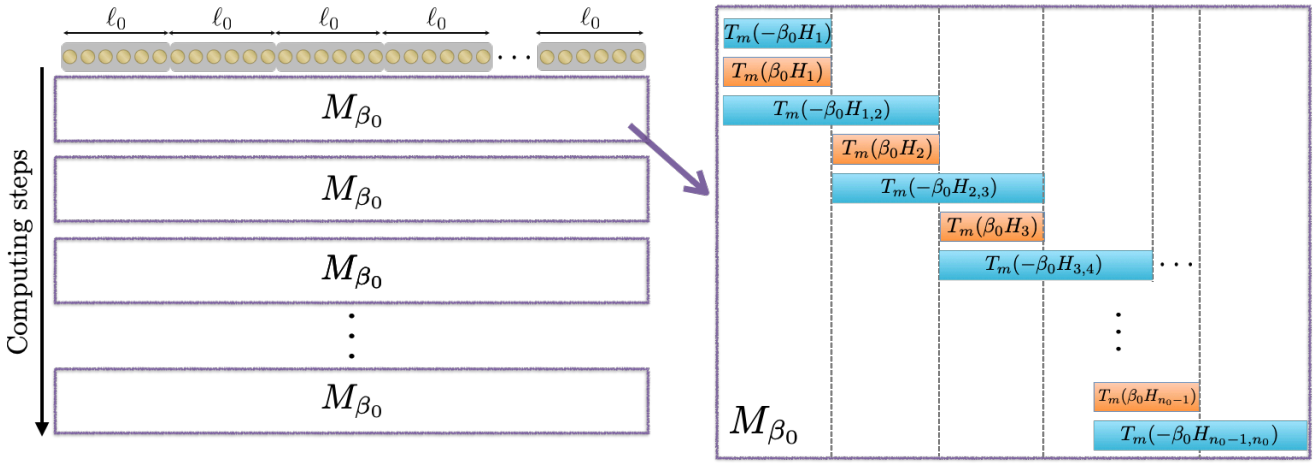

FIG. 1. Our algorithm proceeds by iterated approximations of $e^{-\beta_0 H}$, performed β/β_0 times. In each step, we approximate the Gibbs operator $e^{-\beta_0 H}$ by the operator M_{β_0}. For this, we establish a decomposition of $e^{-\beta_0 H}$ as a product of operators shown on the right-hand side. This uses an imaginary-time version of the Lieb-Robinson bound and the Taylor truncation of the exponential function.

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