Locally accurate matrix product approximation to thermal states

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Abstract

In one-dimensional quantum systems with short-range interactions, we prove that a thermal state at inverse temperature $\beta = O(1)$ has a matrix product representation with bond dimension $e^{\tilde{O}(\sqrt{\beta \log(1/\epsilon)})}$ such that all local properties are approximated to accuracy ϵ.

1 Introduction

One of the most fundamental statements in quantum statistical mechanics is that the state at temperature $T = 1/\beta$ is described by the density matrix

$$\sigma_\beta := e^{-\beta H}/Z, \quad Z := \operatorname{tr} e^{-\beta H}, \tag{1}$$

where Z is the partition function of the Hamiltonian H. In a system of N spins or qudits with local dimension d, σ_β is a square matrix of order d^N. From a computational point of view, it is highly desirable to encode σ_β with a small number of parameters.

Here we focus on one-dimensional systems with short-range interactions. In a remarkable sequence of papers [1–4], σ_β is proved to be efficiently approximated by a matrix product operator (MPO) [5, 6]. Let $\tilde{O}(x) := O(x \log x)$. The state-of-the-art result is

Theorem 1 ([4]). *There exists an MPO ρ with bond dimension*

$$e^{\tilde{O}\left(\beta^{2/3} + \sqrt{\beta \log(N/\epsilon)}\right)} \tag{2}$$

such that $\|\sigma_\beta - \rho\|_1 \le \epsilon$, where $\|X\|_1 := \operatorname{tr}\sqrt{X^\dagger X}$ denotes the trace norm.

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Remark. See Refs. [1–3] for analogues of this theorem in two and higher spatial dimensions.

In practice, we may not have to increase the bond dimension with the system size N. An extreme example is the infinite imaginary time-evolving block decimation algorithm [7], which yields a translation-invariant matrix product representation of thermal states directly in the thermodynamic limit. It is empirically observed that a constant bond dimension is sufficient for computing expectation values of local observables. This observation cannot be explained by Theorem 1, where the bond dimension (2) grows with the system size N and diverges in the thermodynamic limit $N \to +\infty$.

We prove that there exists an MPO with bond dimension

$$e^{\tilde{O}\left(\beta^{2/3}+\sqrt{\beta \log(1/\epsilon)}\right)} \tag{3}$$

such that all local properties of σ_β are approximated to accuracy ϵ. For $\beta = O(1)$, the bond dimension (3) is sub-polynomial in $1/\epsilon$, i.e., $o(1/\epsilon^c)$ for an arbitrarily small constant $c > 0$.

2 Results

Consider a chain of N spins or qudits with local dimension d.

Definition 1 (matrix product operator [5, 6])**.** Let $\{\hat{O}_j\}_{j=0}^{d^2-1}$ be a basis of the space of linear operators on the Hilbert space of a spin. Let $\{D_i\}_{i=0}^{N}$ with $D_0 = D_N = 1$ be a sequence of positive integers. An MPO has the form

$$\rho = \sum_{j_1, j_2, \ldots, j_N = 0}^{d^2-1} \left(A_{j_1}^{(1)} A_{j_2}^{(2)} \cdots A_{j_N}^{(N)}\right) \hat{O}_{j_1} \otimes \hat{O}_{j_2} \otimes \cdots \otimes \hat{O}_{j_N}, \tag{4}$$

where $A_{j_i}^{(i)}$ is a matrix of size $D_{i-1} \times D_i$. Define $\max_{0 \le i \le N} D_i$ as the bond dimension of the MPO ρ.

Consider a local Hamiltonian

$$H = \sum_{i=1}^{N-1} H_i, \quad \|H_i\| = O(1), \tag{5}$$

where H_i represents the nearest-neighbor interaction between spins at positions $i, i+1$, and $\|\cdot\|$ denotes the operator norm. The thermal state σ_β at inverse temperature β is given by Eq. (1).

Theorem 2. *There exists an MPO ρ with bond dimension (3) such that*

$$|\operatorname{tr}(\sigma_\beta \hat{O}) - \operatorname{tr}(\rho \hat{O})| \le \epsilon \tag{6}$$

for any local observable $\hat{O}$ with $\|\hat{O}\| \le 1$.

Proof. We will purify σ_β. We introduce a second (auxiliary) copy of the system. Spins in the original and auxiliary systems are labeled by $1, 2, \dots, N$ and $\bar{1}, \bar{2}, \dots, \bar{N}$, respectively. Let $\{|j\rangle\}_{j=0}^{d-1}$ be the computational basis of the Hilbert space of a spin, and

$$|\Psi\rangle := \frac{e^{-\beta H/2} \otimes I}{\sqrt{Z}} \bigotimes_{i=1}^{N} |\psi\rangle_i, \quad |\psi\rangle_i := \sum_{j=0}^{d-1} |j\rangle_i |j\rangle_{\bar{i}}, \tag{7}$$

where $|\psi\rangle_i$ is an (unnormalized) maximally entangled state of spins i and $\bar{i}$. By construction, $|\Psi\rangle$ is normalized and is a purification of $\sigma_\beta = \mathrm{tr}_a(|\Psi\rangle\langle\Psi|)$, where tr_a denotes the partial trace over the auxiliary system. Combining every pair of spins $i, \bar{i}$ into a composite spin of local dimension d^2, we obtain a chain of N composite spins. Let $i|i+1$ be a cut separating the first i and the last $N-i$ composite spins.

Lemma 1 (Eq. (83) of Ref. [4])**.** *Let $\lambda_1 \geq \lambda_2 \geq \cdots$ be the Schmidt coefficients of $|\Psi\rangle$ across the cut $i|i+1$ in non-ascending order. Then,*

$$\sum_{j>Q_\delta} \lambda_j^2 \leq \delta \quad \text{for} \quad Q_\delta := e^{\tilde{O}\left(\beta^{2/3} + \sqrt{\beta \log(1/\delta)}\right)}. \tag{8}$$

Using this lemma and Lemma 4 in Ref. [8], we obtain an MPO $\tilde{\rho}$ with bond dimension Q_δ^2 such that

$$|\langle\Psi|\hat{O}|\Psi\rangle - \mathrm{tr}(\tilde{\rho}\hat{O})| = O(\sqrt{\delta}) \tag{9}$$

for any local observable $\hat{O}$ with $\|\hat{O}\| \leq 1$. As tracing out the auxiliary system does not increase the bond dimension, $\rho := \mathrm{tr}_a \tilde{\rho}$ is an MPO on the original system with bond dimension Q_δ^2. We complete the proof by letting ϵ be the right-hand side of Eq. (9). □

Remark. Recall that $\tilde{\rho}$ is a locally accurate approximation (9) to the purification $|\Psi\rangle$ of σ_β. Since (pure) matrix product states (MPS) [9, 10] are more favorable than MPO in both theory [11] and practice [12], one might prefer $\tilde{\rho}$ to be an MPS. This can be achieved by using the main results of Refs. [13–15] instead of Lemma 4 in Ref. [8] at the price of weakening the upper bound (3) on the bond dimension of ρ to $e^{\tilde{O}(\beta^{2/3} + \sqrt{\beta \log(1/\epsilon)})}/\epsilon$.

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Recently, I became aware of a related work by Alhambra and Cirac [16], which constructed locally accurate tensor network approximations to thermal states and time-evolution operators in any spatial dimension. Specializing to thermal states in one dimension, my methods and results are significantly different from theirs. Their proof consists of two steps:

1. Construct local approximations assuming exponential decay of correlations.

2. Merge local approximations using the "averaging trick" of Refs. [13, 15, 17].

The proof of Theorem 2 uses neither of these ingredients. Different from Eq. (5) in Result 1 of Ref. [16], the bound (3) does not depend on the correlation length and is sub-polynomial in $1/\epsilon$ for $\beta = O(1)$. This solves an open problem in the conclusion section of Ref. [16].

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