Efficient description of many-body systems with Matrix Product Density Operators

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Matrix Product States form the basis of powerful simulation methods for ground state problems in one dimension. Their power stems from the fact that they faithfully approximate states with a low amount of entanglement, the “area law”. In this work, we establish the mixed state analogue of this result: We show that one-dimensional mixed states with a low amount of entanglement, quantified by the entanglement of purification, can be efficiently approximated by Matrix Product Density Operators (MPDOs). In combination with results establishing area laws for thermal states, this helps to put the use of MPDOs in the simulation of thermal states on a formal footing.

Complex interacting quantum many-body systems cannot be understood without carefully assessing the structure of their quantum correlations, that is, entanglement. This is the key insight behind the Density Matrix Renormalization Group (DMRG) method for the simulation of one-dimensional (1D) systems [1], and it has later allowed to explain DMRG as a variational method over the manifold of Matrix Product States (MPS) [2,3]. This understanding has in turn triggered generalizations of the method for instance to the simulation of time evolution, excitation dynamics, thermal states, to the development of methods for the simulation two- and higher-dimensional systems, gauge theories, and so forth [2,3].

The success of MPS-based methods stems from the fact that MPS faithfully approximate the relevant states, in particular low-energy states of physical systems. The reason for this is deeply rooted in the entanglement structure of those systems: Ground states and low-lying excited states of gapped local Hamiltonians obey an area law for the entanglement entropy – that is, for any contiguous region A, the entanglement $E(A : A^c)$ between A and its complement $A^c$ is bounded by the length of the boundary $\partial A$, $E(A : A^c) \leq \text{const} \times |\partial A|$ (in particular, this is a constant in 1D) [9,10]. Even for critical systems, this behavior is at most logarithmically violated, $E(A : A^c) \leq \text{const} \times \log |A|$ (with $|A|$ the number of sites in $A$). This is a very special property, since the vast majority of quantum many-body states has essentially maximum entanglement, i.e., a volume law [11]. This demonstrates that it is precisely the area law scaling of the entanglement which characterizes the physically relevant “corner” of Hilbert space.

In order to succinctly characterize those states, it is thus necessary to understand the structure of states with limited entanglement, such as an area law or with an only logarithmic increase. It has been found that this is precisely captured by Matrix Product States (MPS)

$$|\phi_D\rangle = \sum_{i_1,\ldots,i_N=1}^d A_{i_1i_1}^{[1]} A_{i_2i_2}^{[2]} \cdots A_{i_Ni_N}^{[N]} |i_1,\ldots,i_N\rangle \quad (1)$$

(here for a chain of $N$ $d$-level spins), where the $A_{ik}^{[k]}$ are $D \times D$ matrices, except for $A_{ik}^{[1]}$ and $A_{ik}^{[N]}$ which are $1 \times D$ and $D \times 1$ matrices, respectively. On the one hand, any MPS obeys an area law by construction. On the other hand, it has been shown that any state which obeys a suitable area law for the entanglement can be faithfully approximated by an MPS, that is, with a $D$ which only grows polynomially in the system size $N$ and the desired accuracy (in contrast to the Hilbert space dimension $d^N$) [12,13]. This clarifies why MPS are well suited to describe ground states and excitations of quantum many-body systems, allowing for efficient simulations.

For thermal states, or more generally mixed states, the situation is much less clear. Again, we can ask the same two key questions: First, what is the structure of entanglement, or more generally correlations, in thermal states of physical systems – in particular, is there some analogue to the area law? And if yes, second: Given a mixed state $\rho$ which obeys an area law, what is the structure of $\rho$, and in particular, can it be well approximated by a Matrix Product Density Operator (MPDO)

$$\sigma_D = \sum A_{i_1j_1}^{[1]} A_{i_2j_2}^{[2]} \cdots A_{i_Nj_N}^{[N]} |i_1,\ldots,i_N\rangle \langle j_1,\ldots,j_N| \quad (2)$$

(where the sum runs over $i_k,j_k = 1,\ldots,d$, and the $A_{ik}^{[k]}$ are as before)? The problem is further impeded by the fact that for mixed states there exists a whole zoo of different entanglement measures which are often not related in a simple fashion. As it turns out, the first of those questions has been addressed previously: It has been shown that thermal states of local Hamiltonians obey an area law for the mutual information, which quantifies both quantum and classical correlations in the system [14]. The second question, however – relating entanglement scaling and approximability by MPDOs – is yet open, and this is what the present work deals with.

In this paper, we show that also for mixed states, a suitable family of entanglement area laws – even with a logarithmic correction – implies that the state can be efficiently approximated by MPDOs. Specifically, given a mixed state $\rho$ on a chain of $N$ $d$-level spins, we prove that
if there exist constants $c > 0$ and $0 < \lambda < 1$ such that the $\alpha$-Rényi entanglement of purification $E_{p,\alpha}$ (defined below) \[15\] satisfies

$$E_{p,\alpha}(A : A^c) \leq c \log N \quad \text{for} \quad \alpha = \frac{\lambda}{5 \log_2 N}, \tag{3}$$

then $\rho$ can be efficiently approximated by an MPDO $\sigma_D$: As long as the bond dimension $D$ scales polynomially, $D = N^\kappa$ for any $\kappa > \frac{2c}{5 \lambda}$, the error $\varepsilon := \|\rho - \sigma_D\|_1$ in trace norm goes to zero super-polynomially in $N$ (i.e., faster than any inverse polynomial) \[16\]. By using the trace norm – which exactly bounds the error in expectation values of arbitrary bounded observables (with largest eigenvalue 1) – we obtain a bound on the error incurred in arbitrary simulations of physical processes. This establishes that MPDOs are precisely the framework needed to faithfully describe mixed states which obey an entanglement area law of the form above.

The proof will on the one side follow the approach in the pure state case \[12\]. On the other side, we need to deviate from it at some key steps. The reason is that we require a good approximation in trace norm, which – unlike the 2-norm – does not induce a scalar product, which in turn is essential to build norm-preserving projections. At the same time, we cannot bound the 2-norm instead: The relative bound $\|\rho\|_2 \leq \sqrt{D} \|\rho\|_1$, with $D = d^N$ the dimension of the total space, is tight (saturated by the maximally mixed state), that is, the trace norm can be exponentially larger in $N$ than the 2-norm, breaking efficiency of the approximation.

We will use the conventional graphical calculus for MPS/MPDOs \[2,8\], where a (mixed) many-body state is denoted as a box with legs (double legs denote ket+bra), Fig. 1(a), and an MPDO is expressed as a tensor network, where tensors are boxes, each leg denotes a tensor index, and connecting legs corresponds to contraction, Fig. 1(b).

Let us briefly sketch the proof strategy: First, we show that for any bipartition, a bound on the entanglement implies that the target state $\rho$ can be well approximated by a low-rank decomposition across that cut. An area law thus implies that $\rho$ has low-rank approximations across every cut. The crucial step will then be to merge these approximations. To start, we will show how to merge two approximations in such a way that (i) we still obtain a good approximation and (ii) the internal structure of the two states is preserved (specifically, existing lower-rank approximations across other cuts), as this allows us to iterate the procedure. In a final step, we then show how to nest this merging procedure in such a way as to obtain a good MPDO approximation of the target state $\rho$.

We start by defining the $\alpha$-Rényi entanglement of purification $E_{p,\alpha}(\rho_{AB})$ \[15\]. For a bipartite state $\rho_{AB}$, it is given by

$$E_{p,\alpha}(\rho_{AB}) = \min_{\psi} E_{\alpha}(\braket{\psi}{\rho_{AB}}), \tag{4}$$

where the minimum is taken over all purifications $|\psi\rangle_A A'BB'$ of $\rho_{AB}$, i.e. $\tr_{A'B'}|\psi\rangle_A = \rho_{AB}$, and $E_{\alpha}(\braket{\psi}{\rho}) = S_{\alpha}(\tr_B \rho_B |\psi\rangle_A \langle \psi|)$, with $S_{\alpha}(\rho) = \frac{1}{1-\alpha} \log(\tr^{\alpha} \rho)$. The $\alpha$-Rényi entanglement entropy quantifying the pure state entanglement between $AA'$ and $BB'$. For the remainder of this paper, we restrict to $0 \leq \alpha < 1$.

A key result from the pure state case \[12\] is that a small $E_{\alpha}(\braket{\psi}{\rho})$ implies a rapid decay of the Schmidt coefficients, and thus there exists a low-rank approximation to $|\psi\rangle$: Concretely, for any $D_p$ there exists a $|\chi_{D_p}\rangle = \sum_{i=1}^{D_p} |\chi_i^A\rangle_{AA'} |\chi_i^R\rangle_{BB'}$ such that

$$\eta := 1 - |\braket{\psi}{\chi_{D_p}}|^2 \leq \left( \frac{1 - \alpha}{D_p} \exp\left[ E_{p,\alpha}(\rho_{AB}) \right] \right)^{\frac{1}{1-\alpha}} \tag{5}$$

(and thus $D_p$ scales as an inverse polynomial in the error $\eta$). This is equivalent to

$$||\psi\rangle - |\chi_{D_p}\rangle||_1 \leq 2\sqrt{1 - \braket{\psi}{\chi_{D_p}}} \leq 2\sqrt{\eta} \tag{6}$$

with $\| \cdot \|_{1}$ the trace norm (i.e. the sum of the singular values) \[17\]. By tracing $A'B'$, and using the fact that tracing (as a completely positive trace preserving map) is contractive under the trace norm, we arrive at

$$\delta := ||\rho_{AB} - \sigma_D||_1 \leq 2\sqrt{\eta} \tag{7}$$

for some

$$\sigma_D = \sum_{i,j=1}^{D_p} A_{ij} \otimes B_{ij} \tag{8}$$

with rank $D = D_p^2$ (where $A_{ij} = \tr_{A'} |\chi_i^A\rangle \langle \chi_i^A|$ and $B_{ij} = \tr_{B'} |\chi_i^R\rangle \langle \chi_j^R|$).

Let us now turn towards a spin chain of length $N$ whose state $\rho$ obeys an area law, that is, there is an $E_{\alpha}^\max$ such that $E_{p,\alpha}(\rho_{AB}) \leq E_{\alpha}^\max$ for any bipartition $A = 1, \ldots, L$, $B = L + 1, \ldots, N$. Combining Eqs. (7) and (8), we have that for each cut, there exists a rank $D = D_p^2$ decomposition of the form \[8\] with trace norm error

$$\delta \leq 2\sqrt{\eta} \leq 2 \left( \frac{1 - \alpha}{E_{\alpha}^\max} \right)^{\frac{1}{1-\alpha}}.$$ \[9\]

What remains to be seen is whether it is possible to merge these different low-rank approximations. However,

![FIG. 1. (a) Tensor notation of density matrix $\rho$: Each pair of legs denotes the ket and bra index at one site. (b) Tensor network for MPDO, Eq. (2). Legs denote indices, connected lines contraction (summation) of indices, corresponding to the matrix products in Eq. (2).](image-url)
at this point we can no longer use the purifications to resort to the pure state result, since the optimal purifications (minimizing $E_{p,\alpha}$) for different cuts need not be related [18]. We thus require a different approach.

To start, consider a bipartite state $\rho \equiv \rho_{AB}$ (obtained by blocking sites), a truncated approximation

$$\sigma_1 = \sum_{i=1}^{D} \hat{A}_i \otimes B_i , \quad \|\rho - \sigma_1\| \leq \delta_1 ,$$  

and another approximation $\sigma_2$,

$$\|\rho - \sigma_2\| \leq \delta_2 ,$$

obtained e.g. by truncating across a different cut. Let us now try to connect those two approximations. To this end, consider a (not necessarily orthogonal) projection $P_1$ onto $\text{span}\{\hat{A}_i\}$, $P_1(A_i) = A_i$, which can be written as $P_1(X) = \sum_{i=1}^{D} \hat{A}_i \text{tr}[(\hat{A}_i)^\dagger X]$ for some basis $\hat{A}_i = \sum_{i=1}^{D} c_{ik} \hat{A}_k$ of $\text{span}\{A_i\}$ and some (dual) matrices $\hat{A}_i$ satisfying $\text{tr}[(\hat{A}_i)^\dagger \hat{A}_j] = \delta_{ij}$. $P_1$ can be naturally embedded into the full space as

$$P_1(X) = \sum_{i=1}^{D} \hat{A}_i \otimes \text{tr}_A[(\hat{A}_i \otimes I_B)^\dagger X] .$$  

Now consider

$$P_1(\sigma_2) = \sum_{i,k=1}^{D} c_{ik} A_k \otimes \text{tr}_A[(\hat{A}_i \otimes I_B)^\dagger \sigma_2] ,$$

see Fig. 2a. First, it also has rank $D$ across the cut; second, the left part is spanned by $A_k$, and thus inherits the structure of the left part of $\sigma_1$; and third, the right part is obtained from $\sigma_2$ by tracing its left part with $(\hat{A}_i)^\dagger$, and thus inherits the structure of the right part of $\sigma_2$. In particular, if $\sigma_1$ and $\sigma_2$ have parts on the left and right, respectively, which are already in Matrix Product form, both of these are inherited by $P_1(\sigma_2)$, see Fig. 2b. We can then iterate this scheme, starting from truncations at individual cuts, to obtain an MPDO approximation.

What is the approximation error of the merged truncation $P_1(\sigma_2)$? Using $P_1(\sigma_1) = \sigma_1$ from [18], we have

$$\|P_1(\sigma_2) - \rho\|_1 \leq \|P_1(\sigma_2) - P_1(\sigma_1)\|_1 + \|P_1(\sigma_1) - \rho\|_1 \leq \|P_1(\sigma_2 - \sigma_1)\|_1 + \|\sigma_1 - \rho\|_1 \leq \|P_1(X)\|_1 + \delta_1 ,$$

(14)

with $X := \sigma_2 - \sigma_1$, $\|X\|_1 \leq \delta_1 + \delta_2$. Starting from (12), a series of elementary inequalities [19] gives

$$\|P_1(X)\|_1 \leq \sum_{i=1}^{D} \|\hat{A}_i\|_1 \|\hat{A}_i\|_\infty \|X\|_1 .$$  

(15)

To keep $\|P_1(X)\|_1$ small, we thus ideally want to choose $\hat{A}_i$ and $\hat{A}_i'$ such that $\|\hat{A}_i\|_1 = \|\hat{A}_i\|_\infty = 1$ (this is optimal as $\delta_{ij} = \text{tr}[(\hat{A}_i')^\dagger \hat{A}_j] \leq \|\hat{A}_i\|_1 \|\hat{A}_j\|_\infty$). It turns out that such $\{\hat{A}_i\}$, $\{\hat{A}_i'\}$ indeed exist, a standard result in functional analysis [20]. Choose a so-called Auerbach basis of the normed space $A = \text{span}\{A_i\}$ with norm $\|\cdot\|_1$, that is, a basis $\{\hat{A}_i\}$ together with a set of linear functionals $\hat{a}_i^* : A \to \mathbb{C}$ such that $\hat{a}_i^*(\hat{A}_j) = \delta_{ij}$ and $\|\hat{A}_i\| = \|\hat{a}_i^*\| = 1$ (such a basis always exists) and extend the bounded functional $\hat{a}_i^*$ to a bounded functional $\text{tr}[(\hat{A}_i')^\dagger \cdot]$, $\|\hat{A}_i\|_\infty = 1$, whose existence is guaranteed by the Hahn-Banach theorem.

By inserting these $\{\hat{A}_i\}$, $\{\hat{A}_i'\}$ in Eq. (15), we arrive at $\|P_1(X)\|_1 \leq D \|X\|_1$, which together with (14) and $\|X\|_1 \leq \delta_1 + \delta_2$ yields

$$\|P_1(\sigma_2) - \rho\|_1 \leq (D + 1)\delta_1 + D\delta_2 .$$

(16)

That is, we have merged the two approximations $\sigma_1$ and $\sigma_2$, with new error as above; if both $\delta_1, \delta_2 \leq \delta$, the new error is at most $(2D + 1)\delta$.

At this point, we can start concatenating truncations using (10). However, we cannot do this sequentially as one would do for the 2-norm (where one can choose $P_1$...
the orthogonal projection for which \(|P_1(X)| \leq |X|\); note that this yields an alternative proof for the result of Ref. [12]: The prefactor \((2D + 1)\) would grow exponentially with the number of steps, rendering the bound useless. To overcome this issue, we choose a renormalization-like procedure, where we concatenate the cuts in a tree-like fashion, as illustrated in Fig. 3, using Eq. (10) in each step. One can readily check that each step doubles the number of cuts and multiplies the error with \((2D + 1)\); if the number of cuts is not a power of 2, we can start some branches of the tree later, or we can pad the spin chain with trivial (uncorrelated) spins. For a chain of length \(N\), this scheme thus requires \(K = \lceil \log_2(N - 1) \rceil \leq (\log_2 N) + 1\) steps, and thus incurs a total error of

\[\varepsilon = (2D + 1)^K \delta \leq (2D + 1)^{\log_2 N + 1} \delta.\]  

(17)

We are now at the point where we can combine our results: Combining Eqs. (9) and (17) yields

\[\varepsilon \leq 2(2D + 1)^{\log_2 N + 1} \left(1 - \alpha \right) e^{E_{\text{max}}/D^{1/2}} \frac{1}{2^N}.\]  

(18)

If we now – following Eq. (3) – choose

\[\alpha = \frac{\lambda}{5 \log_2 N}, \quad e^{E_{\text{max}}/D^{1/2}} = N^c, \quad \text{and} \quad D = N^\kappa,\]  

(19)

with \(0 < \lambda < 1, \kappa > \frac{2c}{\log_2 N}\), we have [using \(1 - \alpha \leq 1, \frac{1}{2^N} \geq 2 \log_2 N/\lambda, 2D + 1 < 3D, \text{and} \ N^\kappa/D^{1/2} \leq 1\]

\[\varepsilon \leq 2(3D)^{\log_2 N + 1} \left(\frac{N^c}{D^{1/2}}\right)^{2 \log_2 N} \]  

(20)

\[\leq 6D \left(\frac{3N^c}{D^{1/2}}\right)^{\log_2 N} = 6N^c \left(\frac{3}{N^\kappa}\right)^{\log_2 N} \rightarrow 0\]  

(21)

with \(\Delta = \frac{1}{\lambda}(\kappa(1 - \lambda) - 2c) > 0\), which thus goes to zero super-polynomially as \(N \to \infty\). This completes the proof of our result.

In summary, in this work we have established when MPDOs can efficiently describe quantum many-body systems. We have derived conditions which a state \(\rho\) has to fulfill such that it can be approximated by an MPDO with a polynomial bond dimension. In particular, we have shown that for a sequence of density operators \(\rho\) on a spin chain of length \(N\), an entanglement area law implies an efficient approximability of \(\rho\) by MPDOs. More concretely, we have considered a family of area law bounds for the Rényi entanglement of purification which limit the quantum correlations to grow at most logarithmically with the system size \(N\); in this setting, we have found that there exist MPDO approximations to \(\rho\) with a bond dimension which grows polynomially in the system size \(N\), and for which the approximation error decreases faster than any inverse polynomial in \(N\). This shows that MPDOs provide a faithful approximation to density operators which satisfy an area law, and are thus well suited for the numerical simulation as well as analytical study of such systems.

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[16] Note that due to the monotonicity of the α-Rényi entropy.
in $\alpha$, we can also choose any smaller $\alpha$ in (3).

[17] This is readily checked by working in the two-dimensional space spanned by the two vectors; note that $|\chi_D\rangle$ need not be normalized.

[18] Different purifications are related by a unitary on the purifying system $A'B'$, which however mixes $A'$ and $B'$ and thus changes the entanglement properties.

[19] Specifically,

$$\|P_1(X)\|_1 \leq \sum \|\hat{A}_i \otimes \text{tr}_A((\hat{A}'_i \otimes \mathbb{1})^T X)\|_1$$

$$= \sum \|\hat{A}_i\|_1 \|\text{tr}_A((\hat{A}'_i \otimes \mathbb{1})^1 X)\|_1$$

$$(\ast) \leq \sum \|\hat{A}_i\|_1 \|((\hat{A}'_i \otimes \mathbb{1})^1 X)\|_1$$

$$\leq \sum \|\hat{A}_i\|_1 \|\hat{A}'_i \otimes \mathbb{1}\|_{\infty} \|X\|_1$$

$$\leq \sum \|\hat{A}_i\|_1 \|\hat{A}'_i\|_{\infty} \|X\|_1,$$

where $(\ast)$ uses the contractivity of the partial trace.

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